# ELECTRON MOBILITY IN RANDOMLY LOCATED HARD-CORE SCATTERERS

by

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SUMMARY

Kubo's formulation of irreversible quantum statistics is applied to electron mobility. In the weak coupling limit the approach to equilibrium is shown to be characterized, in the lowest order, by a relaxation time. With the use of Coopersmith wave functions for hard-core interactions a characteristic relaxation time is derived which to "all orders" is independent of the external (small) driving force. For the specific application to mobility the general theory yields the known results of semi-classical kinetic theory at high temperature and low density. For the region of lower temperature and higher density the theory gives qualitative agreement with the anomalous drop in mobility found by Levine and Sanders for electrons in low temperature helium. However, lack of quantitative agreement indicates a need for further work on the problem.

## ABSTRACT

Kubo's formulation of irreversible quantum statistics is applied to electron mobility. In the weak coupling limit the approach to equilibrium is shown to be characterized, in the lowest order, by a relaxation time. With the use of Coopersmith wave functions for hard-core interactions a characteristic relaxation time is derived which to "all orders" is independent of the external (small) driving force. For the specific application to mobility the general theory yields the known results of semi-classical kinetic theory at high temperature and low density. For the region of lower temperature and higher density the theory gives qualitative agreement with the anomalous drop in mobility found by Levine and Sanders for electrons in low temperature helium. However, lack of quantitative agreement indicates a need for further work on the problem.

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# I. INTRODUCTION

It has long been realized that the quantum mechanical analogue to the Boltzmann equation contained two assumptions of limited and even questionable validity.[1] These are the repeated random phase approximation (RPA) and the relaxation time assumption (RTA) Recently several authors have worked at developing a general transport theory that would avoid these assumptions. Van Hove chose to start with the derivation of the master (Pauli) equation and showed that RPA could, for various physically reasonable potentials, be replaced by a much weaker condition.[2] A number of attempts have also been made starting from the Liouville equation governing the density matrix $\rho$. Greenwood derived an equation for conductivity in a metal which avoided the use of RPA.[3] This formula was evaluated by Edwards for a metal with randomly located impurities to yield the usual solution to the Boltzmann equation.[4] Lax also developed a formal theory which avoids use of RPA. For the case of a weak scattering perturbation (weak-coupling limit) and without RTA he obtained the usual transport result and the Nyquist theorom.[5] Kohn and Luttinger have also shown the validity of the quantum mechanical Boltzmann Eq.

in the weak coupling limit without resorting to RPA or RTA. They carried their work to third order in the coupling strength parameter, and for a periodic lattice with impurities restricted to lattice sites found deviations from standard theory which appear to play a role in the Hall effect.[6]

Kubo also treated irreversible processes starting from the Liouville equation.[7] He developed a formal theory using neither RPA nor RTA. Kubo's theory bears much the same relationship to Irreversible Statistical Mechanics as does the partition function to equilibrium theory. It is an exact, formal theory with (to my knowledge) no questionable assumptions and quite often is rather difficult to evaluate. This theory has been applied by Nakano to conductivity in metals who showed that it gives the Gruneissen formula if one introduces RTA.[8] Chester and Thellung have taken Kubo's formal theory and applied it to elastic scattering in a metal.[9] For the weak coupling limit they obtained results identical with those of the quantum Boltzmann theory with neither RPA nor RTA.

In the present work we calculate electron mobility based on the formal theory developed by Kubo. Neither RPA nor RTA are used. The weak coupling limit is considered briefly in lowest order. Our primary concern, however, is the calculation of electron mobility to "all

orders" in the presence of randomly located hard-core scatterers. We shall see that in both instances the approach to a steady state is actually characterized by a single relaxation time which we derive, not assume.

Our choice of a model based on random hard-sphere scatterers corresponds most closely to the situation in helium vapor. For low energy electrons, helium has a positive scattering length, no Ramsauer effect and the electron-atom interaction is adequately characterized by a spherically symmetric hard-core repulsion.[10]

Electron mobility in helium gas has been experimentally investigated at various times since the early 1920s at temperatures ranging from $77^{o}$ K to $300^{o}$ K.[11] The results of these experiments have been effectively explained by classical kinetic theory. Recently, there has been interest in electron mobility in low temperature helium gas. This was motivated by measurements in liquid helium where it was found that an electron formed a stable dense complex with very low mobility. This led to a prediction that such a complex would also be stable in helium gas at sufficiently low temperature and high density. Measurements to test this hypothesis were made by Levine and Sanders at temperatures near $4^{o}$ K and densities of the order of $10^{21}$ atoms/$cm^{3}$.[12] Under these conditions the mobility was found to be almost four orders of magnitude lower than that obtained from classical

kinetic theory of free electrons. A theory based on formation of a correlated (bubble) state was developed for this high density-low temperature phenomenon, but it failed to account for the transition region at lower density.

A quantum-mechanical consideration of the properties of a free electron experiencing hard-core repulsion in an ideal gas was made by Coopersmith in a calculation of the equilibrium free energy.[13] By using Kubo's quantum mechanical formulation for mobility, we extend this work to the study of a non-equilibrium property. The first order results of this effort have been previously reported[14] and are reviewed in this work in the course of development of the full theory.

All work will be done in units with $\hbar = m = 1$ .

## II. MOBILITY - GENERAL THEORY

The mobility $\mu$ of an electron in the direction of an external electric field E is given by[1]

$$\mu = E^{-1} tr\,(v_z \Delta\rho) \tag{2.1}$$

where tr is a trace and $v_z$ is the electron velocity along E. $\Delta\rho$ is the difference between the total density matrix $\rho_T$ and the unperturbed (E=0) density matrix $\rho$,

$$\Delta\rho = \rho_T - \rho \tag{2.2}$$

The Hamiltonian $H_T$ for an electron in the presence of N scattering centers can be correspondingly divided into

$$H_T = H + \Delta H \tag{2.3}$$

where

$$H = \frac{p^2}{2} + \sum_{i=1}^{N} V_i \tag{2.4}$$

$$\Delta H = -ze\mathcal{E} \tag{2.5}$$

and

$$V_i \equiv V(\vec{r}_{e,i}) = V(\vec{r}_i - \vec{r}_e) \tag{2.6}$$

As mentioned in the first section, Kubo started from the Liouville equation

$$i\,\frac{d\rho_T}{dt} = [H_T, \rho_T] \tag{2.7}$$

and for a weak external perturbation obtained the linearized adiabatic solution

$$\Delta\rho = -i\,Z^{-1}\int_0^{t_E} dt\; e^{-itH}\,[\Delta H, e^{-\beta H}]\,e^{itH} \tag{2.8}$$

where $t_E$ is the length of time the system has been acted on by $\Delta H$ and the equilibrium density matrix is given by

$$\rho = Z^{-1}\exp(-\beta H) \tag{2.9.a}$$

$$Z = tr\,\exp(-\beta H) \tag{2.9.b}$$

As expressed in equation (2.8) $\Delta\rho$ is an average (integral) over the length of time the system is acted on by the perturbing force. The averaging is done to the Heisenberg representation of the commutator of the perturbation and the equilibrium density matrix. A derivation of equation (2.8) is given in Appendix A.

Combining equations (2.1) to (2.9) gives

$$\mu = i e Z^{-1} \mathrm{tr} \int_0^{t_E} dt\, e^{-itH} [\gamma, e^{-\beta H}]\, e^{itH} \rho_{\vec{0}} \qquad (2.10)$$

This equation will be the starting point for the present work.

Kubo actually extended the formal development of the theory by interchanging the trace and the time integral. The resulting integrand (including the trace) he identified as the response function. This response function can then be treated as an average, with the trace defining the averaging process. It is this response function that Kubo and others have used as the starting point for their calculations.[2] While this procedure has calculational advantages for their work (e.g. cyclic permutation of operators), it does not lend itself to the present work. One consequence of taking the trace first is the elimination of information regarding the specific functional form of the time dependence. Specifically, in the course of calculating $\mu$ we would like to consider the limits of validity of RTA. Since we expect that the relaxation time $\tau$ when it does exist is momentum dependent, $\mu$ is best formulated in a way that displays this dependence explicitly. We have sufficient freedom to achieve this since the trace makes the choice of representation

arbitrary. In light of the above comments the obvious procedure is to work in the momentum representation and retain the trace for the last step in the calculation. Some simplification accrues as a result of the above choice, since $\nu_z$ is diagonal in the momentum representation. This follows from the definition of $\nu_z$ and equations (2.3) to (2.5).

$$\nu_z \equiv i[H_T, z] = i[p^2/2, z] = p_z \qquad (2.11)$$

In the momentum representation the eigenvalue equation is

$$\vec{p}\,|\vec{k}\rangle = \vec{k}\,|\vec{k}\rangle \qquad (2.12.a)$$

and the normalization is

$$\langle \vec{k}|\vec{k}'\rangle = \delta(\vec{k}-\vec{k}'), \qquad \langle \vec{k}|\vec{k}\rangle = \Omega/(2\pi)^3 \qquad (2.12.b)$$

where p is the momentum operator, k its corresponding eigenvalue, $\delta(\vec{k}-\vec{k}')$ the Dirac delta function and $\Omega$ the volume of the system.

The above formulation would yield $\mu$ valid only for a particular specific arrangement of the scattering centers, with explicit dependence on the N position parameters $\vec{r}_j$, $j = 1, 2, \ldots N$. The mobility we actually want is the ensemble (configuration) average over all possible arrangements. For a system of N <u>random</u> (uncorrelated) scatterers

$$\bar{\mu} = \Omega^{-N} \int_{\Omega} \cdots \int \prod_{i=1}^{N} d\vec{r}_i \; \mu(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) \qquad (2.13)$$

where the bar indicates an ensemble average. It will be assumed that the ensemble average commutes with the trace and the integration over t.

In the representation in which p is diagonal, the matrix element $P_{kk}$ arising from equation (3.10) for the case of a free electron (plane wave) with no scatterers present can readily be evaluated as

$$P_{kk} \equiv \langle \vec{k} | e^{-\frac{i t p^2}{2}} [z, e^{\frac{-\beta p^2}{2}}] e^{\frac{i t p^2}{2}} | \vec{k} \rangle$$

$$= \langle \vec{k} | [z, e^{\frac{-\beta p^2}{2}}] | \vec{k} \rangle = i \frac{\partial}{\partial k_z} \langle \vec{k} | e^{\frac{-\beta p^2}{2}} | \vec{k} \rangle$$

$$= -i \beta k_z e^{\frac{-\beta k^2}{2}} \langle \vec{k} | \vec{k} \rangle \qquad (2.14)$$

Combining equations (2.1), (2.3) to (2.5) and (2.8) to (2.14) we have

$$\mu = e \beta z^{-1} \mathrm{Tr} \{ k_z^2 e^{\frac{-\beta k^2}{2}} \int_0^{t_e} dt \, \vec{A} \} \qquad (2.15.a)$$

where

$$A = P_{kk}^{-1} \langle \vec{k} | e^{-itH} [z, e^{-\beta H}] e^{itH} | \vec{k} \rangle \qquad (2.15.b)$$

The bar was introduced as a notation to emphasize the presence in our work of the configuration average. For the remainder of the work we shall omit this symbol with the understanding that configuration averages of A

and $\mu$ are implicit in all discussions and will be explicitly shown in all calculations.

## III. EXPANSION PROCEDURE

We cannot proceed to evaluate equation (2.15) directly. This would require the eigenfunction of H, i.e. the full solution to the N-body problem. Instead, A will be recast as an average of an exponential which, as Kubo has shown lends itself to a cluster-type cumulant expansion.

We start with the matrix element, M, in (2.15)

$$M \equiv \langle \vec{k} | e^{-itH} [\lambda, e^{-\beta H}] e^{itH} | \vec{k} \rangle \tag{3.1}$$

$$= \langle \vec{k} | e^{-it\left(\frac{p^2}{2} + \sum_{j=1}^{N} V_j\right)} [\lambda, e^{-\beta\left(\frac{p^2}{2} + \sum_{j=1}^{N} V_j\right)}] e^{it\left(\frac{p^2}{2} + \sum_{j=1}^{N} V_j\right)} | \vec{k} \rangle \tag{3.2}$$

Define $G_j(x)$ and $g_j(x)$ by

$$G_j(x) \equiv 1 + g_j(x) \equiv \exp\left(-\int_0^x e^{\frac{p^2 s}{2}} V_j e^{-\frac{p^2 s}{2}} ds\right) \tag{3.3}$$

and the product $G_j(x) G_k(x)$ by

$$G_j(x) G_k(x) \equiv \exp\left[-\int_0^x e^{\frac{p^2 s}{2}} (V_j + V_k) e^{-\frac{p^2 s}{2}} ds\right] \tag{3.4}$$

Note the identity[1]

$$e^{a(b+c)} = e^{ab} \exp\left(\int_0^a e^{-bs} c\, e^{bs}\, ds\right) \tag{3.5}$$

which is especially useful when $[b,c] \neq 0$ . Upon substitution of equations (3.3) to (3.5) in (3.2)

$$M = \langle \vec{k} | e^{\frac{-it\beta^2}{2}} \prod_{j=1}^{N} G_j(it) \left[ 1, e^{\frac{-\beta\beta^2}{2}} \prod_{j=1}^{N} G_j(\beta) \right] e^{\frac{it\beta^2}{2}} \prod_{j=1}^{N} G_j(-it) | \vec{k} \rangle \qquad (3.6)$$

$$= \langle \vec{k} | e^{\frac{-it\beta^2}{2}} \prod_{j=1}^{N} \{1+g_j(it)\} \left[ 1, e^{\frac{-\beta\beta^2}{2}} \prod_{j=1}^{N} \{1+g_j(\beta)\} \right] e^{\frac{it\beta^2}{2}} \prod_{j=1}^{N} \{1+g_j(-it)\} | \vec{k} \rangle \qquad (3.7)$$

Introduce the levelling operator L with the properties

$$L f^n(x) = \begin{cases} f^n(x) , & n = 0, 1 \\ 0 , & n \geq 2 \end{cases} \qquad (3.8)$$

so that

$$\prod_{j=1}^{N} (1+g_j) \equiv e_L^{\sum_{j=1}^{N} g_j} \qquad (3.9)$$

Equation (3.7) can now be rewritten as

$$M = \langle \vec{k} | e^{\frac{-it\beta^2}{2}} e_L^{\sum_{j=1}^{N} g_j(it)} \left[ 1, e^{\frac{-\beta\beta^2}{2}} e_L^{\sum_{j=1}^{N} g_j(\beta)} \right] e^{\frac{it\beta^2}{2}} e^{\sum_{j=1}^{N} g_j(-it)} | \vec{k} \rangle \qquad (3.10)$$

Now define an average (signified by $\langle\ \rangle$ ) for any product of functions of the three parameters $\pm it$, $\beta$ by

$$\langle f_1(it) f_2(\beta) f_3(-it) \rangle \equiv \langle \vec{k} | e^{\frac{-it\beta^2}{2}} f_1(it) \left[ 1, e^{\frac{-\beta\beta^2}{2}} f_2(\beta) \right] e^{\frac{it\beta^2}{2}} f_3(-it) | \vec{k} \rangle \qquad (3.11)$$

so that M can be written as

$$M = \left\langle e_L^{\sum_{j=1}^{N} g_j(it)} e_L^{\sum_{j=1}^{N} g_j(\beta)} e_L^{\sum_{j=1}^{N} g_j(-it)} \right\rangle \qquad (3.12)$$

Finally introduce an ordering operator $O$ such that even for non-commuting $a$ and $b$,

$$e^{a}e^{b} \equiv O\, e^{a+b} \tag{3.13}$$

and put $M$ in the form

$$M = \langle O\, e^{\sum_i^N [g_i(it) + g_i(\beta) + g_i(-it)]} \rangle \tag{3.14}$$

In this notation $P_{kk}$, equation (2.16), becomes

$$P_{kk} = \langle 1 \rangle \tag{3.15}$$

where $1$ is the identity operator. We have thus demonstrated that $A$ is actually the average of an exponential. It will be useful for us to extend this average and define

$$\mathcal{A}(f_1(it) f_2(\beta) f_3(-it)) \equiv P_{kk} \langle \vec{k} | e^{-\frac{it\hbar^2}{2} f_1(it)} [3, e^{-\frac{\beta\hbar^2}{2} f_2(\beta)}] e^{\frac{it\hbar^2}{2} f_3(-it)} | \vec{k} \rangle \tag{3.16}$$

$\mathcal{A}$ clearly meets two of the requirements of being an average in the cumulant sense. Namely, $\mathcal{A}(1) = 1$ and the moment generating function is well defined. The remaining requirement, that the moments converge will be seen to be satisfied for all moments considered herein. (A summary of the properties of cumulants used in this paper is contained in Appendix B. A more complete and rigorous treatment has been presented by Kubo[2]). Therefore, we can write

$$A = \mathcal{A}\left(0 e_L^{\sum_{i=1}^{N} [g_i(it) + g_i(\beta) + g_i(-it)]}\right)$$

$$= \exp\left\{\mathcal{A}^c\left(0 e_L^{\sum_{i=1}^{N} [g_i(it) + g_i(\beta) + g_i(-it)]} - 1\right)\right\}$$

$$= \exp\left\{\mathcal{A}^c\left(0 L \sum_{n=1}^{\infty} \frac{1}{n!}\left(\sum_{i=1}^{N} [g_i(it) + g_i(\beta) + g_i(-it)]\right)^n\right)\right\} \quad (3.17)$$

where $\mathcal{A}^c$ means the cumulant corresponding to $\mathcal{A}$. Further discussion regarding the cumulant $\mathcal{A}^c$ in the specific context of this work can be found in Appendix C. The following examples demonstrate some properties of the simple (non-cumulant) average $\mathcal{A}$.

$$\mathcal{A}(0 L g_i(\beta) g_i(it)) = \mathcal{A}(g_i(it) g_i(\beta))$$

$$= P_{AA}^{-1} \langle \vec{A} | e^{-it\left(\frac{p^2}{2} + V_i\right)} \left[3, e^{-\beta\left(\frac{p^2}{2} + V_i\right)}\right] e^{\frac{itp^2}{4}} | \vec{A} \rangle \quad (3.18)$$

$$\mathcal{A}(0 L g_i^2(it)) = 0 \quad (3.19)$$

$$\mathcal{A}(0 L g_r(it) g_s(-it) g_{ss}(-it) g_u(\beta) g_q(it) g_{uu}(-it))$$

$$= \mathcal{A}(g_r(it) g_q(it) g_u(\beta) g_s(-it) g_{uu}(-it) g_{ss}(-it))$$

$$= P_{AA}^{-1} \langle A | e^{-it\left(\frac{p^2}{2} + V_s + V_r\right)} \left[3, e^{-\beta\left(\frac{p^2}{2} + V_u\right)}\right] e^{it\left(\frac{p^2}{2} + V_q + V_{uu} + V_{ss}\right)} | \vec{A} \rangle \quad (3.20)$$

Equations (3.18) and (3.19) emphasize the fact that L operates on each class of g-functions separately. This

follows from equations (3.12) and (3.14). Equation (3.20) illustrates the properties of the g-functions as defined in equations (3.3) to (3.5).

Substitution of equation (3.17) in equation (2.15) gives

$$\mu = \rho e Z^{-1} \mathrm{tr}\ \mathcal{H}_3^2 \mathcal{L}^{-\frac{\Delta A}{2}} \int_0^{t_e} dt\ \exp\left\{\mathcal{A}^c (0 \mathcal{L} \sum_n \frac{1}{n!} \left\{\sum_{\rho=1}^{N} \left[g_\rho(\omega) + g_\rho(\rho) + g_\rho(\omega,\rho)\right]\right\}^n)\right\} \quad (3.21)$$

This section started with an expression which contained the Hamiltonian for one electron interacting with N scattering centers. This has been recast in a form which involves instead a summation over n interactions, each involving one electron and n scattering centers.

## IV. WEAK COUPLING

In this section we briefly consider the first order of the cumulant expansion in the weak coupling limit. We will restrict our analysis to the time dependent terms and show that the Kubo formulation yields a relaxation time directly.

Let us consider the time dependent portion $I(t_E)$ of equation (3.21) for $n = 1$ .

$$I(t_E) = \int_0^{t_E} dt\; e^{\mathcal{A}^c\left(OL \sum_{i=1}^{N} [g_i(it) + g_i(-it)]\right)}$$

$$= \int_0^{t_E} dt\; e^{\sum_{i=1}^{N} [\mathcal{A}^c(g_i(it)) + \mathcal{A}^c(g_i(-it))]} \tag{4.1}$$

Recalling the definition of the g-function in (3.3) and using the properties of cumulants we have

$$\mathcal{A}^c(g_i(it)) = \mathcal{A}^c(G_i(it)) - 1 = \mathcal{A}(G_i(it)) - 1 \tag{4.2}$$

and

$$\mathcal{A}^c(g_i(-it)) = [\mathcal{A}^c(g_i(it))]^* \tag{4.3}$$

where the asterisk denotes complex conjugate.

We now evaluate the simple average

$$\mathcal{A}(G_j(it)) = P_{kk}^{-1} \langle \vec{k}| e^{-\frac{itp^2}{2}} \exp\left(-\int_0^{it} d\lambda\, e^{\frac{p^2\lambda}{2}} V_j e^{-\frac{p^2\lambda}{2}}\right)[3, e^{-\frac{\lambda p^2}{2}}] e^{\frac{it\lambda^2}{2}} |\vec{k}\rangle$$

$$= \langle \vec{k}|\vec{k}\rangle^{-1} \langle \vec{k}| \exp\left(-\int_0^{it} d\lambda\, e^{\frac{p^2\lambda}{2}} V_j\, e^{-\frac{p^2\lambda}{2}}\right)|\vec{k}\rangle \qquad (4.4)$$

Expanding the exponential in powers of $V_j$ which is assumed small

$$\mathcal{A}(G_j(it))$$

$$= \langle \vec{k}|\vec{k}\rangle^{-1} \langle \vec{k}| 1 - \int_0^{it} d\lambda\, e^{\frac{p^2\lambda}{2}} V_j e^{-\frac{p^2\lambda}{2}} + \frac{1}{2}\left(\int_0^{it} d\lambda\, e^{\frac{p^2\lambda}{2}} V_j e^{-\frac{p^2\lambda}{2}}\right)^2 + \ldots . |\vec{k}\rangle$$

$$= 1 - it\langle \vec{k}|\vec{k}\rangle \langle \vec{k}|V_j|\vec{k}\rangle$$

$$+ (2\langle \vec{k}|\vec{k}\rangle)^{-1} \int d\vec{k}' |\langle \vec{k}|V_j|\vec{k}'\rangle|^2 \frac{4\sin^2\left[\frac{t}{2}\left(\frac{k'^2}{2} - \frac{k^2}{2}\right)\right]}{\left(\frac{k'^2}{2} - \frac{k^2}{2}\right)^2} \qquad (4.5)$$

Elimination of $\mathcal{A}(G_j(it))$ between equations (4.3) and (4.5) gives

$$\mathcal{A}^c(g_j(it)) + \mathcal{A}^c(g_j(-it)) = \frac{4}{\langle \vec{k}|\vec{k}\rangle} \int d\vec{k}' |\langle \vec{k}|V_j|\vec{k}'\rangle|^2 \frac{\sin^2\left[\frac{t}{2}\left(\frac{k'^2}{2} - \frac{k^2}{2}\right)\right]}{\left(\frac{k'^2}{2} - \frac{k^2}{2}\right)^2} \qquad (4.6)$$

This integral is the same expression that enters the standard derivation of the transition probability in time dependent perturbation theory.[1] We can now introduce a density of states D(k). Since D(k) and $\langle \vec{k}|V_j|\vec{k}'\rangle$ can both be assumed to be slowly varying the integral simplifies considerably and we get

$$A^c(g_i(it)) + A^c(g_i(-it)) = 2\pi \langle \vec{k}|\vec{k}\rangle^{-1} D(k) |\langle \vec{k}|V_i|\vec{k}'\rangle|^2 t \qquad (4.7)$$

If all the interactions are equivalent, then

$$\sum_{i=1}^{N} |\langle \vec{k}|V_i|\vec{k}'\rangle|^2 = N |\langle \vec{k}|V_i|\vec{k}'\rangle|^2 \qquad (4.8)$$

We substitute equations (4.2), and (4.8) and (2.12.b) in (4.1) so that

$$I(t_\epsilon) \sim \int_0^{t_\epsilon} dt\ e^{-t/\tau} \qquad (4.9)$$

where

$$\tau^{-1} = (2\pi)^4 \rho D(k) |\langle \vec{k}|V|\vec{k}'\rangle|^2 \qquad (4.10)$$

and

$$\rho = N/\Omega \qquad (4.11)$$

Actually, the result just obtained is considerably more general than our earlier emphasis on mobility might imply. The conclusions of equations (4.9) and (4.10) were arrived at independent of any considerations involving $\Delta H$. It is, therefore, a quite general property of the linear response by a weakly coupled system that a steady state is approached via an exponential decay of the transient effects. This relaxation proceeds at a rate determined by $\tau$ which thus constitutes the characteristic relaxation time for the system.

## V. MULTIPLE HARD-CORE SCATTERING

After a brief digression in Section IV where we considered the time dependence in the weak coupling limit we return our attention to the hard-core scattering mobility. This section will consider some of the properties of the wave functions used to evaluate the matrix elements that appear in $A$.

The most general matrix element to occur in the expansion of equation (3.21) is

$$\langle \vec{k}_1 | e^{-itH(n_1)} [\,,e^{-\beta H(n_2)}] e^{itH(n_3)} | \vec{k} \rangle \quad , \qquad n_1+n_2+n_3 = n \tag{5.1}$$

where

$$H(n) = \frac{p^2}{2} + \sum_{j=1}^{n} V(r_{je}) \tag{5.2}$$

With the introduction of intermediate states and the judicious choice of formulae for the commutator we will see that much of the calculational work will require evaluation of matrices of the form

$$\langle \vec{k}_1 | e^{-\alpha H(n)} | \vec{k} \rangle$$

$$= (2\pi)^3 \int \cdots \int d\vec{r}_e \, d\vec{r}_{e'} \, e^{-i\vec{k}_1 \cdot \vec{r}_e} e^{i\vec{k} \cdot \vec{r}_{e'}} \langle \vec{r}_e | e^{-\alpha H(n)} | r_{e'} \rangle \tag{5.3}$$

where

The hard-core scattering is represented by the potential

$$V(r) = \begin{cases} \infty , & r \leq a \\ 0 , & r > a \end{cases} \qquad (5.4)$$

where a is the radius of the sphereical region from which the electron is restricted by the scatterer and for helium can be equated with the scattering length. For numerical considerations we will use $a = 6.2 \times 10^{-9}$cm which is the value obtained by O'Malley in an extrapolation of effective-range scattering theory to zero energy.[1]

It is obvious from equation (5.3) that in order to proceed we must first be able to solve

$$H(n)\, \Psi_k(\vec{r}_e ; \vec{r}_1, \vec{r}_2, \cdots \vec{r}_n) = E\, \Psi_k(\vec{r}_e ; \vec{r}_1, \vec{r}_2 \cdots \vec{r}_n) \qquad (5.5)$$

An approximate solution of this equation, with H(n) defined by equations (5.2) and (5.4), was obtained by Coopersmith as part of the free energy study referred to in Section I.[2] The remainder of this section will present the Coopersmith method of solution as well as some of the simplifications which occur when it is used in a cumulant expansion.

The approach underlying the solution is a replacement of equation (5.5) for hard-core interactions by an equivalent boundary value problem. We can alternately consider

$$(\nabla^2+k^2)\,\psi_k(\vec{r}_e;\vec{r}_1,\vec{r}_2\cdots\vec{r}_n)=0 \qquad \text{any } r_{ej}>a \qquad (5.6.a)$$

$$\psi_k(\vec{r}_e;\vec{r}_1,\vec{r}_2\cdots\vec{r}_n)=0 \qquad \text{all } r_{ej}\leq a \qquad (5.6.b)$$

This is a typical two region problem in wave mechanics. $\psi$ satisfies the free particle equation everywhere in space except for n excluded spheres of radius a located at $\vec{r}_j$ . On and within the boundaries of these n spheres $\psi$ must vanish. Because the ensemble average makes the results independent of the particular choice of the n scatterers, we can for convenience, consider the set of scatterers as being labelled 1, 2,... n. The Coopersmith solution then consists of a generalization of the simple scattering solution, i.e. a linear combination of a plane wave and n scattered waves

$$\psi_k(\vec{r}_e;\vec{r}_1,\vec{r}_2\cdots\vec{r}_n)=\frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{r}_{e1}}+\sum_{j=1}^{n}A_j(n)\frac{e^{ikr_{ej}}}{kr_{ej}}\right] \qquad (5.7)$$

The $A_j(n)$ are determined from the n boundary conditions that $\psi$ be zero on the surface of each sphere. The choice of $\exp(i\vec{k}\cdot\vec{r}_{e1})$ for the plane wave part is a matter of convenience and differs from $\exp(i\vec{k}\cdot\vec{r}_e)$ only by a non-physical phase difference. Since everything is expressed solely in relative coordinates we

will use the term coordinate to mean relative coordinate unless specified otherwise.

As indicated earlier, the significant features of low energy hard-core scattering are essentially determined by the S-wave (lowest order partial wave) approximation. This suggests that we perform a multi-centered S-wave expression to determine the coefficients $A_j(n)$. We first expand all terms in equation (5.7), except for $(k r_{e1})^{-1} \exp(i k r_{e1})$, about $\vec{r}_1$, and equate the wave function to zero at $r_{e1} = a$. This process is repeated in turn about each of the remaining (n-1) scattering sites and results in[3]

$$\frac{e^{i\vec{k}\cdot\vec{r}_{ij}} \sin ka}{ka} + A_j(n)\,\frac{e^{ika}}{ka} + \sum_{l=1}^{n}{}' A_l(n)\,\frac{e^{ikr_{ln}} \sin ka}{kr_{ln}a} \qquad (5.8)$$

This is a set of n linear equations, one for each value of j. The prime on the summation indicates the exclusion of the term $l = j$. The solution of this system of equations in determinantal form is the ratio of two nxn determinants where the denominator has elements $a_{st}$ given by

$$a_{st} = \begin{cases} \dfrac{e^{ikr_{st}} \sin ka}{kr_{st}}, & s \neq t \\ e^{ika}, & s = t \end{cases} \qquad (5.9.a)$$

and the numerator has elements $a_{st}$ given by

$$a_{st}^{(j)} = \begin{cases} a_{st} \;, & t \neq j \\ -e^{i\vec{k}\cdot\vec{r}_{sl}} \sin ka \;, & t = j \end{cases} \qquad (5.9.b)$$

In this form each $A_j(n)$ is the sum of $n!$ terms. If we now consider

$$\langle \vec{r}_e | e^{-\alpha H(n)} | \vec{r}_{e'} \rangle$$

$$= \int d\vec{k}\; \psi^*_{\vec{k}}(\vec{r}_e; \vec{r}_1, \vec{r}_2 \cdots \vec{r}_n)\, e^{-\alpha H(n)}\, \psi_{\vec{k}}(\vec{r}_{e'}; \vec{r}_1, \vec{r}_2 \cdots \vec{r}_n) \qquad (5.10)$$

it is apparent that the combination $\psi^*\psi$ involves the sum of more than $(n!)^2$ terms. We, therefore, will attempt to locate and eliminate as many of the non-contributing terms as possible before resorting to explicit evaluation of matrices.

By inspecting the solution for $A_j(n)$ it is seen that the determinants for $A_j(m)$, where $m < n$, are minors of those for $A_j(n)$. The minors are obtained by covering up the rows and columns in the solution of $A_j(n)$ that contain the coordinates of the $(n-m)$ scatterers that appear in $H(n)$ but not $H(m)$. Combining this with the ensemble average employed in $\mathcal{A}$, it follows from the separability feature of cumulants that all terms will vanish unless they contain all $n$

coordinates. This is equivalent to saying (in the standard language of diagrams) that unless these terms contain all $n$ coordinates they will be unlinked.

We also note that every element of the determinants which does contain scatterer coordinates has $\sin(ka)$ as a coefficient. This suggests a further expansion in powers of $ka$ consistent with our mathematical formulation. The gaussian factor $\exp(-\beta k^2/2)$ in equation (5.1) limits the momentum states which contribute to $k$ to the order of $\beta^{-\frac{1}{2}}$ or less. For ambient conditions this gives $ka \lesssim 10^{-1}$ and for the conditions at which Levine and Sanders did their work (see Section I) $ka \lesssim 5\times10^{-3}$. With the expansion in $ka$ equation (5.9) becomes, to lowest order

$$a_{st} = \begin{cases} \dfrac{a\, e^{ikr_{st}}}{r_{st}} , & s \neq t \\ 1 + ika , & s = t \end{cases} \qquad (5.11.a)$$

and

$$a_{st}^{(1)} = \begin{cases} a_{st} , & t \neq j \\ -ka\, e^{i\vec{k}\cdot\vec{r}_{s1}} , & t = j \end{cases} \qquad (5.11.b)$$

Thus, the leading non-vanishing term must have at least $n$ factors of $a$. We will find later

(Section VII) that terms proportional to $a^n$ are also separable and the leading terms will be proportional to $a^{n+1}$ .

## VI. SINGLE SCATTERING MOBILITY

Before proceeding with the full solution for $\mu$ we restrict our attention in this section to the first order effect of hard-core scattering.

Equation (3.21) for $\mu$, with n = 1, is given by

$$\mu = \beta e Z^{-1} \int d\vec{k}\, k_z^2\, e^{-\beta\hbar^2/2m} e^{\sum_{i=1}^{N} A^c(q_i(0))} \int_0^{t_\varepsilon} dt\, e^{\sum_{i=1}^{N} [A^c(q_i(it)) + A^c(q_i(-it))]} \tag{6.1}$$

Our first task is to evaluate the various averages. In first order cumulant averages are equivalent to simple averages, or

$$A^c(q_i(\alpha)) = A(q_i(\alpha)) \quad ; \qquad \alpha = \pm it, \beta \tag{6.2}$$

To evaluate $A$ we need the solution to the Schrödinger equation which for single scattering in the S-wave approximation is

$$\psi_{\vec{k}}(\vec{r}_e; \vec{r}_i) = (2\pi)^{-3/2} \left[ e^{i\vec{k}\cdot\vec{r}_{ei}} - e^{-ika} \sin ka \frac{e^{ikr_{ei}}}{kr_{ei}} \right] \tag{6.3}$$

To second order in ka this becomes

$$\psi_{\vec{k}}(\vec{r}_e; \vec{r}_i) = (2\pi)^{-3/2} \left[ e^{i\vec{k}\cdot\vec{r}_{ei}} - (1 - ika) \frac{a\, e^{ikr_{ei}}}{r_{ei}} \right] \tag{6.4}$$

This leads to the diagonal matrix elements

$$\Omega^{-N}\int\cdots\int\prod_{j=1}^{N} d\vec{r}_j \,\langle\vec{k}|e^{-\alpha\left(\frac{p^2}{2}+V_j\right)}|\vec{k}\rangle$$

$$=(8\pi^3\Omega)^{-1}\int\cdots\int d\vec{r}_j\, d\vec{r}_c\, d\vec{r}_{c'}\, e^{-i\vec{k}\cdot(\vec{r}_c-\vec{r}_{c'})}\langle\vec{r}_c|e^{-\alpha\left(\frac{p^2}{2}+V_j\right)}|r_{c'}\rangle$$

$$=(8\pi^3\Omega)^{-1}\int\cdots\int d\vec{r}_j\, d\vec{r}_c\, d\vec{r}_{c'}\, e^{-i\vec{k}\cdot(\vec{r}_c-\vec{r}_{c'})}\int d\vec{k}'\,\psi^*_{\vec{k}'}(\vec{r}_c;\vec{r}_j)\,e^{-\frac{\alpha k'^2}{2}}\,\psi_{\vec{k}'}(\vec{r}_{c'};r_j)$$

$$=\left[\langle\vec{k}|\vec{k}\rangle-2\pi a\alpha+2(2\pi)^{1/2}a^2\,\frac{\alpha k^2-1}{k}\int_0^{\sqrt{\alpha}k}dx\, e^{\frac{x^2}{2}}e^{\frac{\alpha k^2}{2}}\right]e^{-\frac{\alpha k^2}{2}} \qquad (6.5)$$

With the definition of $\mathcal{A}$ in equation (3.16) we obtain

$$\sum_{j=1}^{N}\left[\mathcal{A}^c(g_j(it))+\mathcal{A}^c(g_j(-it))\right]$$

$$=\frac{-2RA}{K}\left[(K^2T+1)C(KT^{1/2})+(K^2T-1)S(KT^{1/2})+\frac{KT^{1/2}}{\pi^{1/2}}\left(\cos\frac{K^2T}{2}-\sin\frac{K^2T}{2}\right)\right] \qquad (6.6)$$

$$\sum_{j=1}^{N}\mathcal{A}^c(g_j(\beta))=-R\left\{1+\frac{A}{8\pi}\left[(K^{-3}+2K^{-1}-K)\,D(K\beta^{1/2})-(2/\pi)^{1/2}(K^{-2}-1)e^{\frac{K^2}{2}}\right]\right\} \qquad (6.7)$$

where

$$C(x)=\int_0^x dy\,\cos\frac{\pi y^2}{2} \qquad \text{(Fresnel integrals)} \qquad (6.8.a)$$

$$S(x)=\int_0^x dy\,\sin\frac{\pi y^2}{2} \qquad (6.8.b)$$

$$D(x)=\sqrt{\frac{2}{\pi}}\int_0^x dy\, e^{\frac{y^2}{2}} \qquad \text{(Dawson function)} \qquad (6.9)$$

and the following dimensionless variables have been introduced

$$K^2=k^2\beta \qquad (6.10.a)$$

$$T=t/\beta\ ,\ \mathcal{T}=\mathcal{T}/\beta \qquad (6.10.b)$$

$$A = \alpha/\beta^{1/2} \qquad (6.10.c)$$

$$R = 2\pi\rho a\beta \qquad (6.10.d)$$

The intervening steps for the above results are presented in Appendix E.

Expansion of the Fresnel integrals[1] shows that for $K^2T \gg 1$ the RHS of equation (6.6) approaches $T/\mathcal{T}$ where $\mathcal{T} = (2RAK)^{-1}$. Thus we find that, just as in the case of weak coupling, a relaxation time has appeared as a direct consequence of the theory.

If we limit ourselves to $2RA \ll 1$ (low density-high temperature; e.g. one atm. and 300°K) and assume that the gaussian factor restricts the contributing values of the momentum to $K \sim 1$, then in these circumstances $T_E \gg \mathcal{T}$ and the RHS of (6.7) is $\cong 1$. In these circumstances

$$\mu \cong \frac{e e^{-R} \beta^{1/2}}{Z} \int d\vec{K}\, K_1^2 e^{\frac{-K^2}{2}} \int_0^\infty dT\, e^{-2ARKT} = \frac{4e}{3\rho\sigma(2\pi m\theta)^{1/2}} \qquad (6.11)$$

where $m$ is the electron mass, $\theta$ is the product of temperature and the Boltzmann constant and $\sigma$ is the quantum-mechanical low energy hard sphere cross section[2], $\sigma = 4\pi a^2$. The normalization $Z$ was shown by Coopersmith[3] to be given by $Z=\exp(-R)$. Equation (6.11) is exactly the same as the result obtained from classical kinetic theory.[4]

## VII. EXPANSION OF CUMULANTS

In this section we will examine the $n^{th}$ order cumulant expansion and consider the effects upon it arising from the levelling operation, cumulant separability and the thermodynamic limit.

Each individual cumulant entering the expansion of equation (3.21)

$$\mathcal{A}^c\left(\sum_n \frac{1}{n!} OL\left\{\sum_{j=1}^{N}\left[g_j(it)+g_j(\beta)+g_j(-it)\right]\right\}^n\right) \qquad (7.1)$$

is necessarily of the form

$$\mathcal{A}^c\left(OL\prod_{k=1}^{n_1} g_{j_k}(it)\prod_{k=1}^{n_2} g_{j_k}(\beta)\prod_{k=1}^{n_3} g_{j_k}(-it)\right) \quad , \quad n_1+n_2+n_3=n \qquad (7.2)$$

An essential feature of cumulants for the considerations in this section is that $\mathcal{A}^c(\prod_{j=1}^{n} g_j)$ is expanded as a sum of products, each of the form $\prod_i' \mathcal{A}(\prod_{k=1}^{n_i} g_{j_k})$ . The prime on $\prod$ indicates that the product is subject to the restriction $\sum_i n_i = n$ . This is discussed in more detail in Appendix B.

Let us first consider those terms where one of the $n_i = n$ and the other two are zero. The levelling operator will equate to zero any $\mathcal{A}$ which contains a repeated subscript. However, some terms will remain

from a cumulant with repeated subscripts provided the repeated subscripts are distributed among the $\mathcal{A}$'s such that there is no repetition of a subscript within a single $\mathcal{A}$ . (See Appendix C). As defined in equation (3.16), $\mathcal{A}$ has a normalization proportional to $\langle \vec{A} | \vec{A} \rangle \sim \Omega^{-1}$ . The ensemble average of $\mathcal{A}(\prod_{i=1}^{n} g_{l_i})$ introduces a factor proportional to $\Omega^{-n_1+1}$ . Thus each term of the $n^{th}$ order cumulant is proportional to $\Omega^{-n}$ . As mentioned earlier, the dependence of $\mathcal{A}^c$ on a particular set of scatterers is eliminated when the configuration average is taken. Thus, the $n$ summations over the subscripts are just the number of ways of choosing the different subscripts out of $N$ . This is $N(N-1)\ldots(N-n+1)$ when all $n$ subscripts differ, and $N(N-1)\ldots(N-m+1)$ when only $m, (m<n)$, different subscripts appear. Now we combine the results for $N$ and $\Omega$ above and go to the limit of large $N$ and $\Omega$ , $N/\Omega = \rho$ . For the case where all $n$ subscripts differ we have $(N/\Omega)^n = \rho^n$ . However, when there are only $m$ different subscripts we have $N^m/\Omega^n$ which in the limit of large $N$ and $\Omega$ is vanishingly small. Such terms need not be considered further.

It remains to consider the terms for which two (or all three) of the $n_i$ are non-zero. If one or more subscripts are repeated within a single set of

$n_j$ subscripts there will be no contributions. This follows from the same reasoning as above and these terms will not be considered further. This leaves those terms in which there are only $m < n$ different subscripts, but with no subscript repeated within any single $n_j$ . In this instance the same considerations used above show that there are terms proportional to $\rho^m$ . Since there are $n$ scattering interactions involved, the non-separable (linked) term of lowest order in $a$ must have at least $n$ factors of $a$ . If $n > m+1$ these terms are of lower order in $a$ than we consider here. If $n=m+1$, these terms are in general separable in the cumulant sense as is shown in Appendix H. The exceptions are $\mathcal{A}^c(g_j(it)g_j(\beta))$ and its complex conjugate $\mathcal{A}^c(g_j(\beta)g_j(-it))$ with contributions $\sim \rho a^2$ . $\mathcal{A}^c(g_j(it)g_j(-it))$ is zero because it contains an odd function to be integrated over a symmetric region. The former terms are considered further in Section VIII and Appendix I. The latter term is shown to vanish in Appendix J. As a consequence of the above we can rewrite equation (3.21) as

$$\mu = \beta e Z^{-1} \mathrm{tr}\left\{ h_i \, e^{-\frac{\beta A^k}{2}} \int_0^{t_E} dt \right.$$

$$\times \exp\left\{ A^c \left( \sum_n \frac{1}{n!} L \left\{ \left[ \sum_{j=1}^{N} g_j(it) \right]^n + \left[ \sum_{j=1}^{N} g_j(\beta) \right]^n + \left[ \sum_{j=1}^{N} g_j(-it) \right]^n \right\} \right.\right.$$

$$\left.\left. + \frac{1}{2} \sum_{j=1}^{N} \left[ g_j(it) g_j(\beta) + g_j(\beta) g_j(-it) \right] \right) \right\} \Bigg\} \qquad (7.3)$$

Since most of the complexity of cumulant expansion is present for n=3 we have compiled all n=3 terms in figure 7.1. They are listed together with a summary of the highlights of the above discussion and references to the locations of additional relevant material.

It has also been shown by Coopersmith that another simplification arises from the angular part of the integration required to express the coordinate matrix elements in terms of the wave function, namely, from

$$\int d\theta \sin\theta \, \psi^* \psi \qquad (7.4)$$

From equations (5.7) for $\psi$ and (5.11) for $A_j$ we see that all coordinates enter $\psi^* \psi$ multiplicatively as either spherically symmetric scattered waves, $(kr)^{-1} \exp(\pm ikr)$, or plane waves, $\exp(\pm i\vec{k} \cdot \vec{r})$. Since the only angular dependence in $\psi \psi$ is in the plane waves, the integration of expression (7.4) transforms the plane wave part of $\psi^* \psi$ into scattered waves.

$$\int_0^{\pi} d\theta \sin\theta \; e^{\pm i\vec{k}\cdot\vec{r}} = \frac{e^{ikr} - e^{-ikr}}{ikr}$$

Thus the exponentials in $\psi^*\psi$ can be written as a single exponential of the sums and differences of coordinates, $\exp(ik\Sigma \pm r_j)$. Considering the various ways of obtaining combination $\Sigma \pm r_j$ leads to the conclusion that all such terms cancel unless they are $\pm\Sigma r_j$, i.e. positive definite or negative definite. Since $\psi^*\psi$ is real these will be expressable as sines and cosines of sums of coordinates.

There are two types of terms which occur in $\psi^*\psi$. They either arise from the product of a plane wave and a scattered wave or the product of two scattered waves. The latter terms must necessarily contain at least one coordinate in the exponential which has the opposite sign from the rest and will cancel those of the former terms in which the argument of the trigonometric function is not positive definite. An explicit demonstration is given in Appendix D for the case n=2.

## VIII. EVALUATION OF AVERAGES

In this section we present the explicit results necessary for the evaluation of the exponential in equation (7.3).

$$\mathcal{A}^c\Big(\sum_n \frac{1}{n!} L\Big\{\Big[\sum_{j=1}^{N} g_j(\alpha)\Big]^n + \Big[\sum_{j=1}^{N} g_j(\beta)\Big]^n + \Big[\sum_{j=1}^{N} g_j(-\alpha)\Big]^n\Big\} + \frac{1}{2}\sum_{j=1}^{N}\big[g_j(\alpha)g_j(\beta) + g_j(\beta)g_j(-\alpha)\big]\Big) \qquad (8.1)$$

We will first consider the averages and then the summations of the above expression.

Let us introduce the notation $\mathcal{A}_n(\alpha)$ to represent $\mathcal{A}\big(\prod_{j=1}^{n} g_j(\alpha)\big)$ and $\mathcal{A}_n(\alpha; a^m)$ to represent that part of $\mathcal{A}\big(\prod_{j=1}^{n} g_j(\alpha)\big)$ which is proportional to $a^m$. In this notation

$$\mathcal{A}^c\Big(L\Big[\sum_{j=1}^{N} g_j(\alpha)\Big]^n\Big) = N(N-1)\cdots(N-n+1)\,\mathcal{A}_n^c(\alpha) \qquad (8.2)$$

From the arguments of Section V we know that $m \geq n$. Two values of $m$ will actually be needed, namely $m=n$ and $m=n+1$. The terms $m=n$ alone are insufficient because $\mathcal{A}_n^c(\alpha; a^n) = 0$, as will be seen below. However, this does not make $\mathcal{A}_n(\alpha; a^n)$ irrelevant as it does contribute to the expansion of $\mathcal{A}_n^c(\alpha; a^{n+1})$.

Let us consider

$$\mathcal{A}_n(it) = (P_{\vec{k}\vec{k}}\,\Omega^n)^{-1}\int\cdots\int\prod_{j=1}^{n} d\vec{r}_j \,\langle\vec{k}|e^{-it\left(\frac{p^2}{2}+\sum_{j=1}^{n}V_j\right)}[3, e^{-\beta\frac{p^2}{2}}]e^{\frac{it}{2}p^2}|\vec{k}\rangle \qquad (8.3)$$

$$= (\Omega^n\langle\vec{k}|\vec{k}\rangle)^{-1}\, e^{\frac{it\vec{k}^2}{2}}\int\cdots\int\prod_{j=1}^{n} d\vec{r}_j \,\langle\vec{k}|e^{-it\left(\frac{p^2}{2}+\sum_{j=1}^{n}V_j\right)}|\vec{k}\rangle \qquad (8.4)$$

$$= \Omega^{-n+1} e^{\frac{it\vec{k}^2}{2}}\int\cdots\int\prod_{j=1}^{n} d\vec{r}_j\, d\vec{r}_{e'}\, d\vec{r}_{e}\, e^{-i\vec{k}\cdot(\vec{r}_e-\vec{r}_{e'})}\langle\vec{r}_e|e^{-it\left(\frac{p^2}{2}+\sum_{j=1}^{n}V_j\right)}|\vec{r}_{e'}\rangle \qquad (8.5)$$

The contribution to $\mathcal{A}_n(it;a^n)$ from the coordinate matrix element is

$$4\pi(-1)^n a^n n!\int_0^\infty dk\, k\, e^{-\frac{it\vec{k}^2}{2}}\frac{\sin k(r_{e1}+r_{12}+\cdots r_{n-1,n}+r_{ne'})}{r_{e1}\,r_{12}\cdots r_{n-1,n}\,r_{ne'}} \qquad (8.6)$$

so that

$$\mathcal{A}_n(it;a^n) = (-2\pi a\, it/\Omega)^n \qquad (8.7)$$

while the contribution to $\mathcal{A}_n(it;a^{n+1})$ is

$$4\pi(-1)^n a^{n+1} n!\, n\int_0^\infty dk\, k^2 e^{-\frac{it\vec{k}^2}{2}}\frac{\cos k(r_{e1}+r_{12}+\cdots r_{n-1,n}+r_{ne'})}{r_{e1}\,r_{12}\cdots r_{n-1,n}\,r_{ne'}} \qquad (8.8.a)$$

and

$$4\pi(-1)^n a^{n+1} n!\sum_{m=1}^{n-1}\int_0^\infty dk\, k\, e^{-\frac{it\vec{k}^2}{2}}\frac{\sin k(r_{e1}+r_{12}+\cdots r_{m-1,m}+r_{me'}+r_{m,m+1}+r_{m+1,m+2}+\cdots r_{n-1,n}+r_{nm})}{r_{e1}\,r_{12}\cdots r_{m-1,m}\,r_{me'}\,r_{m,m+1}\,r_{m+1,m+2}\cdots r_{n-1,n}\,r_{nm}} \qquad (8.8.b)$$

so that

$$A_n(it;a^{n+1}) = \frac{2\pi a(-2\pi\rho a)^n}{(2\pi)^{1/2}}\left\{e^{\frac{it\hbar^2}{2}}\frac{\partial}{\partial(it)}\int_0^{\sqrt{it}} d\lambda\,(it-\lambda^2)^n e^{\frac{\hbar^2}{2}(\lambda^2-it)}\right.$$

$$\left. -\int_0^{\sqrt{it}} d\lambda\left[(it)^{n-1}-(\lambda^2)^{n-1}\right]e^{\frac{\hbar^2\lambda^2}{2}}\right. \qquad (8.9)$$

Equation (8.3) is $A_n(it)$ as defined in equation (3.16). Equation (8.4) follows from equations (2.12) and (2.14). Equation (8.5) is the transformation from momentum to coordinate representation. Expressions (8.6) and (8.8) follow from the discussion of Section V. (Additional details may be found in Appendices D and F. (8.6) and (8.8) are extensions to general n of expressions (F.3) and (F.4) for n=3). The integrals in R.H.S. of equation (8.5), with integrands given by expression (8.6) and (8.8), are evaluated in Appendix G.

In a similar manner we have

$$A_n(\beta) = (P_{4\pi}\Omega^N)^{-1}\int\cdots\int\prod_{j=1}^{N} d\vec{r}_j\,\langle\vec{k}|e^{\frac{-it\rho^2}{2}}[3, e^{-\beta(\frac{\rho^2}{2}+\sum_{j=1}^{n}V_j)}]\,e^{\frac{it\rho^2}{2}}|\vec{k}\rangle$$

$$= \left(\Omega^{n+1}\frac{\partial}{\partial k_z}e^{\frac{-\beta k^2}{2}}\right)^{-1}\int\cdots\int\prod_{j=1}^{n} d\vec{r}_j\,d\vec{r}_{e'}\,d\vec{r}_e\cdot e^{-i\vec{k}\cdot(\vec{r}_e-\vec{r}_{e'})}\langle\vec{r}_e|e^{-\beta(\frac{\rho^2}{2}+\sum_{j=1}^{n}V_j)}|r_{e'}\rangle \qquad (8.10)$$

$$A_n(\beta;a^n) = (-2\pi a\beta/\Omega)^n \qquad (8.11)$$

$$A_n(\beta;a^{n+1}) = \frac{2\pi a(-2\pi\rho a)^n}{(2\pi)^{1/2}} \frac{\partial}{\partial k_i} e^{-\frac{\beta k^2}{2}} \frac{\partial}{\partial k_j}\left\{ e^{\frac{\beta k^2}{2}} \frac{\partial}{\partial\beta} \int_0^{\sqrt{\beta}} d\lambda \left[ (\beta-\lambda^2)^n - \beta^{n-1}+(\lambda^2)^{n-1} \right] e^{\frac{k^2}{2}(\lambda^2-\beta)} \right\} \quad (8.12)$$

The last average we have to evaluate is

$$A(q_j(it)q_j(\rho)) = (P_{kk}\Omega^N)^{-1} \int\cdots\int \prod_{j=1}^{N} d\vec{r}_j \langle \vec{k}| e^{-it(\frac{p^2}{2}+V_j)} [3, e^{-\beta(\frac{p^2}{2}+V_j)}] e^{it\frac{p^2}{2}} |\vec{k}\rangle \quad (8.13)$$

$$= -i(P_{kk}\Omega)^{-1} e^{\frac{it k^2}{2}} \int d\vec{r}_j \langle \vec{k}| e^{-it(\frac{p^2}{2}+V_j)} e^{-\beta(\frac{p^2}{2}+V_j)} \int_0^{\beta} d\lambda\, e^{\lambda(\frac{p^2}{2}+V_j)} p_i\, e^{-\lambda(\frac{p^2}{2}+V_j)} |\vec{k}\rangle \quad (8.14)$$

$$= \frac{2a^2(2\pi)^{N/2} e^{\frac{\beta k^2}{2}}}{\beta\Omega} \left[ \int_0^{\beta} d\lambda \frac{(\beta^2-\lambda^2)}{(\beta-\lambda)^{3/2}} e^{\frac{-k^2\lambda^2}{2}} + \beta^2 \int_0^{it} d\lambda\, (\beta+\lambda^2) e^{\frac{k^2\lambda^2}{2}} \right. \quad (8.15)$$

The identity[1] for the commutator of an operator A with the density matrix

$$[A, e^{-\beta H}] = -i e^{-\beta H} \int_0^{\beta} d\lambda\, e^{\lambda H} \dot{A} e^{-\lambda H} \quad (8.16)$$

was used to go from equation (8.13) to equation (8.14) where $\dot{A}$ is the time derivative of A. The transition from equation (8.14) to (8.15) is presented in detail in Appendix H.

The remaining averages in expression (8.1) are obtained by complex conjugation, since

$$A_n(-it) = [A_n(it)]^* \quad (8.17)$$

$$\mathcal{A}(g_j(\beta)\, g_j(-it)) = [\mathcal{A}(g_j(it)\, g_j(\beta))]^* \tag{8.18}$$

We note that the cumulant separability of $\mathcal{A}_n(\alpha; a^n)$ for $n > 1$ follows from equations (8.8) and (8.11) which show that

$$\mathcal{A}_n(\alpha; a^n) = [\mathcal{A}_1(\alpha; a)]^n \tag{8.19.a}$$

We also note that

$$\mathcal{A}_1^c(it; a) + \mathcal{A}_1^c(-it; a) = \mathcal{A}_1(it; a) + \mathcal{A}_1(-it; a) = 0 \tag{8.19.b}$$

$$\mathcal{A}_1^c(\beta; a) = \mathcal{A}_1(\beta; a) = -2\pi\beta a/\Omega \tag{8.19.c}$$

It now remains to perform the various summations indicated in (8.1). As discussed in Section VII the n-fold summation over $j$ from 1 to N, gives $N(N-1)\ldots(N-n+1)$ which goes to $N^n$ in the limit of large $N$. Thus, performing these summations has the effect of replacing $\Omega^{-n}$ by $\rho^n$ in (8.8), (8.11), (8.14), and (8.19.c).

The final procedure remaining is the summation over $n$ of the cumulant expansion.

$$\sum_{n=1}^{\infty} \frac{1}{n!} \mathcal{A}_n^c(it; a^{n+1}) = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{q=1}^{n} (-1)^{q-1}(q-1)! \sum_{\substack{q \\ \sum_{j=1} m_j = n}} \prod_{j=1}^{q-1} P\, \mathcal{A}_{m_j}(it; a^{m_j})\, \mathcal{A}_{m_q}(it; a^{m_{q+1}}) \tag{8.20}$$

$$= \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{q=0}^{n} \frac{n!}{(n-q)!} A_{n-q}(it; a^{n-q+1}) \sum_{p=0}^{q} (-1)^p p! \sum_{\substack{\Sigma \lambda m_\lambda = q \\ \Sigma m_\lambda = p}} \frac{[A_1(it;a)]}{\prod_\lambda (\lambda!)^{m_\lambda} m_\lambda!} \tag{8.21}$$

$$= \sum_{n=1}^{\infty} \sum_{q=0}^{n} \frac{(-1)^q}{q!(n-q)!} A_{n-q}(it; a^{n-q+1}) [A_1(it;a)] \tag{8.22}$$

$$= \frac{4\pi a R}{(2\pi)^{3/2}} \int_0^{\sqrt{it}} d\lambda \, e^{\frac{R^2\lambda^2}{2}} \left[ 1 + (2R + R^2)(it - \lambda^2) e^{R\lambda^2} e^{R(it-\lambda^2)} - e^{R\lambda^2} - 2e^{R\lambda^2} \right] \tag{8.23.a}$$

$\exp(-\beta k^2/2)$

similarly

$$\sum_{n=1}^{\infty} \frac{1}{n!} A_n^c(\beta; a^{n+1})$$

$$= \frac{4\pi a R}{(2\pi)^{3/2}} e^{-\alpha k^2} \frac{\partial}{\partial k_z} \int_0^{\sqrt{\beta}} d\lambda \, e^{\frac{R^2\lambda^2}{2}} \left[ 1 + (2R + R^2)(\beta - \lambda^2) e^{R\lambda^2} e^{R(\beta-\lambda^2)} - e^{R\lambda^2} - 2e^{R\lambda^2} \right] \tag{8.23.b}$$

In writing equation (8.20), the standard expression for the cumulant expansion (see App. B) has been modified by separating out one $A$ to demonstrate explicitly the proportionality to $a^{n+1}$ and inserting $P$ to indicate that we must include all the permutations of the remaining $A$'s that satisfy this proportionality. Equation (8.21) is a rearrangement of the summation which contains explicitly the combinatorial factor arising from $P$ and also makes use of equation (8.19). Equation (8.22) follows from equation (8.21) as a consequence of the properties of the Stirling number of the second kind (see Appendix H). Equation (8.23) is a straighforward summation of equation (8.22) with the $A$'s eliminated by using equations (8.7) and (8.9).

The remaining cumulant is

$$\sum_{j=1}^{N} \mathcal{A}^{c}(g_j(r)g_j(\rho)) = \sum_{j=1}^{N}\left[\mathcal{A}(g_j(r)g_j(\rho)) - \mathcal{A}(g_j(r))\,\mathcal{A}(g_j(\rho))\right] \qquad (8.24)$$

The second term of R.H.S. is smaller than the first by a factor of $\Omega^{-1}$ since each $\mathcal{A}$ is $\sim\Omega^{-1}$ and there is only a single summation $\sim N$. Therefore, the second term is negligible in the limit of large $N$ and $\Omega$.

In the preceding sections we saw that the cumulant expansion is equivalent to an expansion in $\rho$ and the S-wave approximation with its related expansion in $ka$ introduced a further expansion into each cumulant. Our approximation scheme now consists of locating the leading term in $a$ for each power of $\rho$ and summing these over all powers of $\rho$. In this sense we are solving the problem to "all orders."

## IX. RESULTS AND DISCUSSION

As a consequence of the work in Sections V, VII and VIII, equation (3.21) for the mobility can be expressed in terms of cumulant averages by

$$\mu = e\beta Z^{-1} tr\{A_j^2 e^{-\frac{\beta k^2}{2}\int_0^{t_E} dt}$$

$$\times exp\left[\sum_n \frac{N^n}{n!}\{A_n^c(it;a^{n+1}) + A_n^c(\beta;a^{n+1}) + A_n^c(-it;a^{n+1})\}\right.$$

$$\left. + \frac{N}{2}\{A(g_j(it)g_j(\beta)) + A(g_j(\beta)g_j(-it))\} + NA(\beta;a)\right]\} \tag{9.1}$$

Upon replacement of the cumulant averages by the explicit expressions obtained in Section VIII, we have

$$\mu = \frac{2e\beta^{1/2}}{3(2\pi)^{1/2}}\int_0^\infty dK\, K^4 e^{-\frac{K^2}{2}} e^{-f(\beta,R,K)}\int_0^{T_E} dT\, e^{-F(\beta,R,K,T)} \tag{9.2}$$

where

$$f = f_1 + f_2 \tag{9.3}$$

$$f_1 \equiv \sum_n \frac{N^n}{n!} A_n^c(\beta;a^{n+1})$$

$$= AR\{(K^{-1}+K^{-3})D(K) - (Q_-^{-1}+Q_-^{-3})D(Q_-) + (Q_+ - 2Q_+^{-1} - Q_+^{-3})D(Q_+)$$

$$+ \sqrt{2/\pi}\left[2RK^{-2}Q_+^{-2}e^{\frac{K^2}{2}} - (1-Q_+^{-2})e^{\frac{Q_+^2}{2}}\right]\} \tag{9.4}$$

and $f_2$ is the time independent part of the second term on the RHS of equation (8.1)

$$f_2 \equiv 2(2\pi)^{3/2} RA e^{\frac{K^2}{2}} \int_0^1 d\lambda \, \frac{1+\lambda}{(1-\lambda)^{3/2}} \, e^{\frac{-K^2\lambda^2}{2}} \tag{9.5}$$

Similarly

$$F = F_1 + F_2 \tag{9.6}$$

$$F_1 \equiv \sum_n^- \frac{N^n}{n!} \left[ \mathcal{A}_n^{\,c}(it; a^{n+1}) + \mathcal{A}_n^{\,c}(-it; a^{n+1}) \right]$$

$$= 2AR\Big\{ TQ_+ \left[ S(Q_+\sqrt{T/\pi}) + C(Q_+\sqrt{T/\pi}) \right]$$

$$+ K^{-1}\left[ S(K\sqrt{T/\pi}) - C(K\sqrt{T/\pi}) \right] - Q_+^{-1/2}\left[ S(Q_+\sqrt{T/\pi}) - C(Q_+\sqrt{T/\pi}) \right]$$

$$- Q_-^{-1/2}\left[ (\sin RT - \cos RT) C(Q_-\sqrt{T/\pi}) + (\sin RT + \cos RT) S(Q_-\sqrt{T/\pi}) \right]$$

$$- \sqrt{T/\pi}\,(\sin TQ_+^2 - \cos TQ_+^2)\Big\} \tag{9.7}$$

$$F_2 = 2(2\pi)^{1/2} RA e^{\frac{K^2}{2}} \int_0^{iT} d\lambda \, (\beta+\lambda)^{-3/2} \, e^{\frac{K^2\lambda^2}{2}} \tag{9.8}$$

and

$$Q_\pm^2 \equiv K^2 \pm 2R \tag{9.9}$$

Equation (9.4) follows from (8.22) and (8.9) while (9.7) follows from (8.22) and (8.7).

It is interesting to note that for all physically reasonable values of the parameters $f_2 \ll f_1$ and $F_2 \ll F_1$. Thus no cumulant with repeated subscripts contributes to the results.

When we expand C(x) and S(x) asymptotically we find that for $Q_+^2 \ll T$

$$F \cong 2RA(R+K^2)^{1/2}T \tag{9.10}$$

In general there is a large region in which this is satisfied. Typical values for a mobility experiment are $10^{-1} < 2RA(R + K^2)^{\frac{1}{2}} < 10^2$ and $10^7 < T_E < 10^{10}$. Thus we again (as in Sections IV and VI) find that after an interval small compared to the duration of the experiment, the transient effects die out and the system approaches a steady state exponentially. We therefore make the identification of the relaxation time as

$$\tau^{-1} = 2RA(R+K^2)^{1/2} \tag{9.11}$$

We note that where $K \gg R$ (e.g. one atm. and 300° K) equation (9.11) reduces to the first order result $\tau = (2RAK)^{-1}$. As before, this relaxation time result was obtained independent of the specific form of $\Delta H$.

Figure 9.1 shows exp(f) as a function of K for selected values of R. In each instance the function looks like a step function with the step located vary near K=0 and the step height dependent on R. For $R \sim 1$ (e.g. one atm. and 300° K), $\exp(f) \cong 1$, as was the case in the first order calculations (see Section IV). The integrations indicated in equation (9.2) were performed numerically using a Simpson's rule for the K integration

and a Gauss-Laguerre procedure for the T integration. In the former it was necessary to assume that the gaussian factor $\exp(-K^2/2)$ provided an adequate cut-off, as $\exp(f)$ becomes strongly divergent for large K. This is a reasonable restriction as the inclusion of large K is equivalent to considering contributions from high energy electrons which is physically unrealistic and contrary to our mathematical restriction $KA \ll 1$ .

Figure 9.2 shows $\mu$ vs. $\rho$ for a temperature of $3.96^{\circ}$ K. The circles are the experimental results obtained by Levine and Sanders. The dashed straight line is the semi-classical theory given by equation (6.11). The broken line is the first order result obtained by numerical integration of equation (6.1) with the $\mathcal{A}$ 's expressed by (6.6) and (6.8). The solid line is the full result obtained by numerical integration of (9.2). Since the integral of (9.2) is a function of the dimensionless parameter $R = 2\pi\rho a\beta$, it follows that the solution at any other temperature (i.e. $\beta$) is a simple translation (in $\rho$) of the above result.

At lower densities the experimental mobility approaches that predicted by the theoretical calculations for free energy. The high density region is understood in terms of the formation of a correlated, or "bubble", state. However, the transition region in which there is a large drop in $\mu$ for a fairly small increase in $\rho$ has

not been explained. Calculations based on a transition from free electron motion to correlated motion predict a transition that is much too sharp.[1] Our calculation indicates a decrease in $\mu$ that is qualitatively correct (i.e. the theoretical and experimental curves have similar slopes) but the result is quantitatively wrong (i.e. it occurs at too low a density). We do not see any modification of the theory or improvement on the hard-sphere model that could cause the theory to coincide quantitatively with the experiments.

It is rather interesting to find that our theory, which considers only free states, yields a mobility which becomes vanishingly small. The severe drop in $\mu$ only appears when all higher order (multiple scattering) terms of the cumulant expansion are included and comes from exp(f) (see figure 9.1) which in turn comes from $[\Delta H, e^{-\beta H}]$ . In the formulation of the theory this is the interaction of the external perturbing force with the equilibrium ($\Delta H=0$) density matrix. However, the physical process causing this rapid change in $\mu$ is not clear. One possibility is that our result is somehow related to the Anderson transition[2] whereby conduction goes to zero in certain random systems. Another possibility might be the appearance of some ordering in the system. Both of these suggestions are highly speculative, but do

indicate directions in which this study might be pursued further.

## X. CONCLUSION

We have applied cumulant theory to Kubo's formulation of irreversible quantum statistical mechanics. In the weak coupling limit we saw (Section IV) that in lowest order the approach to steady state is always characterized by a relaxation time. Similarly, for hard core interactions we found that with the use of Coopersmith wave functions we derived a characteristic relaxation time independent of the specific nature of the interaction, $\Delta H$. For the specific application to mobility, $\Delta H = -zeE$, we found that the general theory yielded the well known results of semi-classical theory at high temperature-low density. For the region of lower temperature and higher density the theory was shown to give qualitative agreement with the anomalous results of experiment. However, the quantitative disagreement indicated a need for further work on this problem.

# APPENDIX A

## KUBO'S LINEARIZED ADIABATIC SOLUTION OF THE LIOUVILLE EQUATION[1]

The density operator $\rho_T$ (in the notation of Section II) obeys the Liouville Equation

$$i \frac{d\rho_T}{dt} = [H_T, \rho_T] \tag{A.1}$$

This is expanded as

$$i \frac{d}{dt} (\rho + \Delta\rho) = [H + \Delta H, \rho + \Delta\rho]$$

$$= [H,\rho] + [H, \Delta\rho] + [\Delta H, \rho] + [\Delta H, \Delta\rho] \tag{A.2}$$

The equilibrium density matrix $\rho$ satisfies

$$i \frac{d\rho}{dt} = [H, \rho]$$

and in a linear approximation we can neglect $[\Delta H, \Delta\rho]$ .

Thus

$$i \frac{d}{dt} \Delta\rho = [\Delta H, \rho] + [H, \Delta\rho] \tag{A.3}$$

We now solve for $\Delta\rho$

$$-H\Delta\rho + i\frac{\partial}{\partial t}\Delta\rho + \Delta\rho H = [\Delta H, \rho]$$

$$e^{-itH}\frac{\partial}{\partial t}\left(e^{itH}\Delta\rho e^{-itH}\right)e^{itH} = -i[\Delta H, \rho]$$

$$e^{itH}\Delta\rho e^{-itH} = -i\int_{t_o}^{t} dt'\, e^{it'H}[\Delta H, \rho]e^{-it'H} \qquad \text{(A.4)}$$

where $t_o$ is that time at which $\rho_T(t_o) = \rho$ , $\Delta\rho(t_o) = 0$

This gives

$$\Delta\rho = -i\int_{t_o}^{t} dt'\, e^{-i(t-t')H}[\Delta H, \rho]e^{i(t-t')H} \qquad \text{(A.5)}$$

which with the variable changes $(t-t') \rightarrow t$ and $(t-t_o) \rightarrow t_E$ , becomes

$$\Delta\rho = -i\int_{o}^{t_E} dt\, e^{-itH}[\Delta H, \rho]e^{itH} \qquad \text{(A.6)}$$

# APPENDIX B

## CUMULANTS - GENERAL THEORY[1]

This appendix summarizes the properties of cumulant theory that are used in this work. Cumulants are also sometimes referred to as semi-invariants or (in complex form) characteristics.

The defining equation for the cumulants of $x$ is

$$\mathcal{A}^c(e^{\xi x}-1) = \ln \mathcal{A}(e^{\xi x}) \tag{B.1}$$

where $\mathcal{A}$ is a normalized average and $\mathcal{A}^c$ is the cumulant average corresponding to the simple (non-cumulant) average $\mathcal{A}$. Both sides of the equation (B.1) can be expanded and coefficients of like powers of $\xi$ equated. This leads directly to

$$\mathcal{A}^c(1) = \mathcal{A}(1) = 1 \tag{B.2}$$

$$\mathcal{A}^c(x) = \mathcal{A}(x) \tag{B.3}$$

$$\mathcal{A}^c(x^2) = \mathcal{A}(x^2) - \mathcal{A}^2(x) \tag{B.4}$$

$$\mathcal{A}^c(x^3) = \mathcal{A}(x^3) - 3\mathcal{A}(x^2)\mathcal{A}(x) + 2\mathcal{A}^3(x) \tag{B.5}$$

$$\mathcal{A}^c(x^4) = \mathcal{A}(x^4) - [4\mathcal{A}(x^3)\mathcal{A}(x) + 3\mathcal{A}^2(x^2)] + 12\mathcal{A}(x^2)\mathcal{A}^2(x) - 6\mathcal{A}^4(x) \qquad \text{(B.6)}$$

and so on.

Straightforward extension to multiple variable gives

$$\mathcal{A}^c(e^{\sum_i \xi_i x_i} - 1) = \ln \mathcal{A}(e^{\sum_i \xi_i x_i}) \qquad \text{(B.7)}$$

which yields the following relationships:

$$\mathcal{A}^c(x_1 x_2) = \mathcal{A}(x_1 x_2) - \mathcal{A}(x_1)\mathcal{A}(x_2) \qquad \text{(B.8)}$$

$$\mathcal{A}^c(x_1 x_2 x_3) = \mathcal{A}(x_1 x_2 x_3) - [\mathcal{A}(x_1)\mathcal{A}(x_2 x_3) + \mathcal{A}(x_2)\mathcal{A}(x_1 x_3) + \mathcal{A}(x_3)\mathcal{A}(x_1 x_2)]$$

$$+ 2\mathcal{A}(x_1)\mathcal{A}(x_2)\mathcal{A}(x_3) \qquad \text{(B.9)}$$

and so on.

A general expression for $\mathcal{A}^c(x_1 x_2 \cdots x_n)$ where no variable is present to a power greater than one is

$$\mathcal{A}_c^c(x_1 x_2 \cdots x_n) = \sum_{q=1}^{n} (-1)^{q-1}(q-1)! \sum_{\sum_{j=1}^{q} m_j = n} \prod_{j=1}^{q} \mathcal{A}\left(\prod_{k=1}^{m_j} x_{n_k}\right) \qquad \text{(B.10)}$$

The summation in (B.10) means the sum over all possible arrangements of the set of n variables in q subsets.

Much of the utility of cumulant theory in many-body studies comes from its "separability" property which can be stated as follows: A cumulant will be zero if one (or more) of its variables is statistically independent of the other variables.

As an example of separability we consider equation (B.9) with $x_1$, separable. Separability of $x_1$, implies

$$A(x_1 x_2) = A(x_1) A(x_2) \qquad \text{(B.11.a)}$$

$$A(x_1 x_3) = A(x_1) A(x_3) \qquad \text{(B.11.b)}$$

$$A(x_1 x_2 x_3) = A(x_1) A(x_2 x_3) \qquad \text{(B.11.c)}$$

Using equations (B.11) in equation (B.9) gives

$$A'(x_1 x_2 x_3) = A(x_1) A(x_2 x_3) - [A(x_1) A(x_2 x_3) + A(x_2) A(x_1) A(x_3) + A(x_3) A(x_1) A(x_2)]$$

$$+ 2 A(x_1) A(x_2) A(x_3)$$

$$= 0 \qquad \text{(B.12)}$$

## APPENDIX C

## CUMULANTS - IN THE PRESENT CONTEXT

The four step prescription for disentangling equation (3.17) is: expand the exponential, order the resulting products, expand the cumulants in terms of the corresponding simple averages, and lastly, apply the levelling operator.

A specific example of this procedure is

$$\mathcal{A}^c\left(0\, e_L^{\sum_{j=1}^{N} g_j} - 1\right)$$

$$= \mathcal{A}^c\left(0L\left\{\left[\sum_{j=1}^{N} g_j\right] + \frac{1}{2!}\left[\sum_{j=1}^{N} g_j\right]^2 + \frac{1}{3!}\left[\sum_{j=1}^{N} g_j\right]^3\right\}\right)$$

$$= \sum_{j=1}^{N} \mathcal{A}^c(0L\, g_j) + \frac{1}{2!}\sum_{j=1}^{N}\sum_{k=1}^{N} \mathcal{A}^c(0L\, g_j g_k)$$

$$+ \frac{1}{3!}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} \mathcal{A}^c(0L\, g_j g_k g_l) \qquad (C.1)$$

where

$$g \equiv g(it) + g(\beta) + g(-it)$$

A typical expression that would require both ordering and levelling might be found in the third term of RHS of equation (C.1) where the ordering would consist of

$$\mathcal{A}^c\{OL\, g_n(p)\, g_n(it)\, g_n(p)\} = \mathcal{A}^c\{L\, g_n(it)\, g_n^2(p)\} \tag{C.2}$$

The RHS of equation (C.2) can be expanded in terms of simple averages by

$$\mathcal{A}^c\{OL\, g_n(p)\, g_n(it)\, g_n(p)\}$$

$$= \mathcal{A}\{L\, g_n(it)\, g_n^2(p)\} - [\mathcal{A}\{L\, g_n(it)\}\mathcal{A}\{L\, g_n^2(p)\} + 2\mathcal{A}\{L\, g_n(p)\}\mathcal{A}\{L\, g_n(it)\, g_n(p)\}]$$

$$+ 2\mathcal{A}\{L\, g_n(it)\}\mathcal{A}^2\{L\, g_n(p)\} \tag{C.3}$$

Finally, application of L to RHS of (C.3) gives

$$\mathcal{A}^c\{OL\, g_n(p)\, g_n(it)\, g_n(p)\} = -2[\mathcal{A}\{g_n(p)\}\mathcal{A}\{g_n(it)\, g_n(p)\} - \mathcal{A}\{g_n(it)\}\mathcal{A}^2\{g_n(p)\}] \tag{C.4}$$

In general, the operator L must be applied <u>after</u> the cumulant has been expanded. In the above example this means that L can be applied to RHS of equation (C.3) but not to RHS of equation (C.2). Otherwise the surviving terms in RHS of equation (C.4) would be lost. In the present work, however, one could safely commute the cumulant expansion and levelling procedures because the surviving terms, as in RHS of equation (C.4), turn out to be negligibly small. This last point is discussed in Section VI.

# APPENDIX D

## TRIGONOMETRIC FUNCTIONS OF COORDINATES

We noted in Section VII that the arguments of the trigonometric functions entering the coordinate matrix elements are all positive definite. We consider this matter further in this appendix which contains an explicit demonstration of the feature for $n=2$.

Before proceeding let us introduce some notation and collect some relations found elsewhere but needed for this presentation

$$a_{st} = \frac{a\, e^{ikr_{st}}}{kr_{st}} \quad , \; s \neq t \qquad ; \; a_{st} = a_{ts} \tag{D.1}$$

$$a_{ss} = i - \tfrac{2}{3} a \tag{D.2}$$

$$A_1(2)\frac{e^{ikr_{e1}}}{kr_{e1}} = \frac{-\begin{vmatrix} 1 & a_{12} \\ e^{-i\vec{k}\cdot\vec{r}_{12}} & 1+a_{22} \end{vmatrix}}{\begin{vmatrix} 1+a_{11} & a_{12} \\ a_{21} & 1+a_{22} \end{vmatrix}} \tag{D.3}$$

$$A_2^*(2)\frac{e^{-ikr_{e2}}}{kr_{e2}} = \frac{\begin{vmatrix} 1+a_{11}^* & 1 \\ a_{21}^* & e^{i\vec{k}\cdot\vec{r}_{12}} \end{vmatrix}}{\begin{vmatrix} 1+a_{11}^* & a_{12}^* \\ a_{22}^* & 1+a_{22}^* \end{vmatrix}} \tag{D.4}$$

$$\int_0^{\pi} d\theta \sin\theta \, e^{\pm i\vec{k}\cdot\vec{r}_{st}} = \frac{e^{ikr_{st}} - e^{-ikr_{st}}}{ikr_{st}} = \frac{a_{st} - a_{st}^*}{a_{ss}} \qquad \text{(D.5)}$$

We will also use the following schematic notation for locating terms in the determinants. A circle at the location of an element indicates that the element contributes to the result when the determinant is expanded.

The angular integration of

$$\langle \vec{r}_e | e^{-\alpha H(2)} | \vec{r}_{e'} \rangle = \int d\vec{k} \; \psi_k^*(\vec{r}_e ; \vec{r}_1, \vec{r}_2) \, e^{-\frac{\alpha k^2}{2}} \psi_k(\vec{r}_{e'} ; \vec{r}_1, \vec{r}_2) \qquad \text{(D.6)}$$

is

$$\int_0^{\pi} d\theta \sin\theta \left[ e^{-i\vec{k}\cdot\vec{r}_{e1}} + A_1^*(2) a_{e1}^* + A_2^*(2) a_{e2}^* \right] \left[ e^{i\vec{k}\cdot\vec{r}_{e'1}} + A_1(2) a_{e'1} + A_2(2) a_{e'2} \right] \qquad \text{(D.7)}$$

Let us consider the particular cross product

$$\int_0^{\pi} d\theta \sin\theta \, e^{-i\vec{k}\cdot\vec{r}_e} A_1(2) a_{e'1} \qquad \text{(D.8)}$$

and look for those terms containing indices 1 and 2 and proportional to $a^2$ and $a^3$ (see Section VII for further discussion of this point). The terms we want are

$$-\int_0^\pi d\theta\ \sin\theta\ e^{-i\vec{k}\cdot\vec{r}_{e1}}\left\{\frac{|_0{}^0|}{|^0{}_0|}+\frac{|^0{}_0|}{|^0{}_0|}\right\}a_{e'1}$$

$$=-\int_0^\pi d\theta\ \sin\theta\ e^{-i\vec{k}\cdot\vec{r}_{e1}}\left\{(-a_{12}e^{-i\vec{k}\cdot\vec{r}_{12}})(1+a_{11})^{-1}(1+a_{22})^{-1}+(1+a_{22})(1-a_{12}^2)^{-1}\right\}a_{e'1}$$

$$=(ika)^{-1}\left[-(a_{e2}-a_{e2}^*)a_{12}a_{e'1}(1-a_{11}-a_{22})+(a_{e1}-a_{e1}^*)a_{12}^2a_{e'1}\right] \qquad (D.9)$$

let us look at the exponentials contained in R.H.S.

$$a_{e2}a_{12}a_{e'1}\Longrightarrow e^{ik(r_{e2}+r_{12}+r_{e'1})} \qquad (D.10)$$

$$a_{e2}^*a_{12}a_{e'1}\Longrightarrow e^{ik(-r_{e2}+r_{12}+r_{e'1})} \qquad (D.11)$$

$$a_{e1}a_{12}^2a_{e'1}\Longrightarrow e^{ik(r_{e1}+2r_{12}+r_{e'1})} \qquad (D.12)$$

$$a_{e1}^*a_{12}^2a_{e'1}\Longrightarrow e^{ik(-r_{e1}+2r_{12}+r_{e'1})} \qquad (D.13)$$

The coordinates in (D.10) and (D.12) are positive definite while (D.11) and (D.13) are not. We will locate the complex conjugate to (D.10) and show how it combines and also the counterpart to (D.11) to show that it cancels

Let us look for $a_{e2}^*a_{12}^*a_{e'1}^*$ . The only other source for $a_{e2}^*$ is from the scattered wave $A_2^*(2)a_{e2}^*$ or

$$\int_0^\pi d\theta\ \sin\theta\ e^{i\vec{k}\cdot\vec{r}_{e'1}}A_2^*(2)a_{e2}^* \qquad (D.14)$$

which gives

$$-\frac{(a_{e11}-a^*_{e11})}{ika}\begin{vmatrix}0 & 0\\ 0 & 0\end{vmatrix} a^*_{e2} \qquad \text{(D.15)}$$

from which we can pick out

$$(ika)^{-1} a^*_{e1}\, a_{12}\, a^*_{e2}\,(1+a_{11}+a_{22}) \qquad \text{(D.16)}$$

The other cross-product of this scattered wave is

$$\int_0^\pi d\theta\, \sin\theta\, A^*_2(2)\, a^*_{e2}\, A_1(2)\, a_{e11} \qquad \text{(D.17)}$$

which gives

$$\int_0^\pi d\theta\, \sin\theta \begin{vmatrix}0 & 0\\ 0 & 0\end{vmatrix} a^*_{e2}\left\{\begin{vmatrix}0 & 0\\ 0 & 0\end{vmatrix} + \begin{vmatrix}0 & 0\\ 0 & 0\end{vmatrix}\right\} a_{e11} \qquad \text{(D.18)}$$

from which we can pick out

$$(ika)^{-1} a^*_{e2}\, a_{12}\, a_{e11} - 2\, a^*_{e2}\, a_{12}\, a_{e11} \qquad \text{(D.19)}$$

Combining the first term of R.H.S of (D.9) with (D.16) and (D.19) we find that the exponentials with ordinates of mixed signs cancel, and we are left with

$$2a^2\left[k^{-1}\sin k(r_{e2}+r_{12}+r_{e11}) - a\cos k(r_{e2}+r_{12}+r_{e11})\right] \qquad \text{(D.20)}$$

# APPENDIX E

## INTEGRALS, FIRST ORDER

Equations (7.6) and (7.7) are obtained as follows:

$$A_t \equiv \sum_{j=1}^{N} \left[ A^c(q_j(it)) + A^c(q_j(-it)) \right]$$

$$= \sum_{j=1}^{N} \left[ A(q_j(it)) + A(q_j(-it)) \right]$$

$$= \sum_{j=1}^{N} \left[ A(G_j(it)) - 1 + A(G_j(-it)) - 1 \right]$$

$$= \sum_{j=1}^{N} (\Omega^N P_{AA})^{-1} \int \cdots \int \prod_{j=1}^{N} dr_j \left[ \langle \vec{A} | e^{-it\left(\frac{p^2}{2} + V_j\right)} \left[ 3, e^{-\frac{\beta p^2}{2}} \right] e^{\frac{it p^2}{2}} | \vec{A} \rangle \right.$$

$$\left. + \langle \vec{A} | e^{\frac{-it p^2}{2}} \left[ 3, e^{-\frac{\beta p^2}{2}} \right] e^{it\left(\frac{p^2}{2} + V_j\right)} | \vec{A} \rangle - 2 P_{AA} \right]$$

$$= \sum_{j=1}^{N} \left\{ (\Omega P_{AA})^{-1} \int dr_j \left[ e^{\frac{it A^2}{2}} \langle \vec{A} | e^{-it\left(\frac{p^2}{2} + V_j\right)} | \vec{A} \rangle + e^{-\frac{it A^2}{2}} \langle \vec{A} | e^{it\left(\frac{p^2}{2} + V_j\right)} | \vec{A} \rangle \right] - 2 \right\}$$

Similarly

$$A_\beta \equiv \sum_{j=1}^{N} A^c(q_j(\beta))$$

$$= \sum_{j=1}^{N} \left[ \left( \Omega \langle \vec{A} | \vec{A} \rangle \frac{\partial}{\partial A} e^{-\frac{\beta A^2}{2}} \right)^{-1} \frac{\partial}{\partial A} \int dr_j \langle \vec{A} | e^{-\beta\left(\frac{p^2}{2} + V_j\right)} | \vec{A} \rangle - 1 \right]$$

Thus we need to evaluate

$$\alpha_{\vec{k}\vec{k}'} \equiv \int d\vec{r}_i \, \langle \vec{k} | e^{-\alpha\left(\frac{p^2}{2} + V_i\right)} | \vec{k}' \rangle$$

$$= \int d\vec{r}_i \int d\vec{r}_e \int d\vec{r}_{e'} \, \langle \vec{k} | \vec{r}_e \rangle \langle \vec{r}_e | e^{-\alpha\left(\frac{p^2}{2} + V_i\right)} | \vec{r}_{e'} \rangle \langle \vec{r}_{e'} | \vec{k}' \rangle$$

$$= (2\pi)^{-3} \int d\vec{r}_i \int d\vec{r}_e \int d\vec{r}_{e'} \, e^{-i\vec{k}\cdot(\vec{r}_e - \vec{r}_{e'})} \langle \vec{r}_e | e^{-\alpha\left(\frac{p^2}{2} + V_i\right)} | \vec{r}_{e'} \rangle$$

where

$$\langle \vec{r}_e | e^{-\alpha\left(\frac{p^2}{2} + V_i\right)} | \vec{r}_{e'} \rangle$$

$$= \int d\vec{k} \; \psi_{\vec{k}}(\vec{r}_e ; \vec{r}_i) \, e^{-\frac{\alpha k^2}{2}} \psi_{\vec{k}}(\vec{r}_{e'} ; \vec{r}_i)$$

$$\cong (2\pi)^{-3} \int d\vec{k} \left[ e^{-i\vec{k}\cdot\vec{r}_{ei}} - (1 + ika) \frac{e^{-ikr_{ei}}}{k r_{ei}} \right] e^{-\frac{\alpha k^2}{2}} \left[ e^{i\vec{k}\cdot\vec{r}_{e'i}} - (1 - ika) \frac{e^{ikr_{e'i}}}{k r_{e'i}} \right]$$

$$\cong (2\pi)^{-3} \int d\vec{k} \; e^{-\frac{\alpha k^2}{2}} e^{-i\vec{k}\cdot(\vec{r}_e - \vec{r}_{e'})}$$

$$- \frac{2}{(2\pi)^2 r_{ei} r_{e'i}} \int_0^\infty dk \left[ ka \sin k(r_{ei} + r_{e'i}) + k^2 a^2 \cos k(r_{ei} + r_{e'i}) \right] e^{-\frac{\alpha k^2}{2}}$$

$$= (2\pi)^{-3/2} e^{-\frac{|\vec{r}_e - \vec{r}_{e'}|^2}{2\alpha}} + \frac{2}{(2\pi)^2 r_{ei} r_{e'i}} \left[ a \frac{d}{d(r_{ei} + r_{e'i})} - a^2 \frac{d^2}{d(r_{ei} + r_{e'i})^2} \right] \left(\frac{2\pi}{\alpha}\right)^{1/2} e^{-\frac{(r_{ei} + r_{e'i})^2}{2\alpha}}$$

Eliminating the matrix element in $\alpha_{kk}$ we have

$$\alpha_{kk} - \Omega \langle \vec{k}|\vec{k}\rangle e^{-\frac{\alpha k^2}{2}}$$

$$= \frac{4\Omega a}{\alpha^{3/4}(2\pi)^{3/2}k^2}\int_0^\infty dr \int_0^\infty dr' \sin kr \sin kr' \left[\frac{\partial}{\partial(r+r')} - a\frac{\partial^2}{\partial(r+r')^2}\right] e^{\frac{-(r+r')^2}{2\alpha}}$$

$$= \frac{\Omega a}{\alpha^{3/4}(2\pi)^{3/2}k^2}\int_0^\infty dx \int_x^\infty dy\, (\cos kx - \cos ky)\left[\frac{\partial}{\partial x} - a\frac{\partial^2}{\partial x^2}\right] e^{\frac{-x^2}{2\alpha}}$$

$$= \frac{2\Omega a}{\alpha^{3/4}(2\pi)^{3/2}k^2}\left[\frac{\partial}{\partial k} - \frac{1}{k}\right]\left\{\frac{\partial}{\partial k}\int_0^\infty dx\, e^{\frac{-\alpha x^2}{2}} \cos kx + a\left[1 + \frac{1}{\alpha}\frac{\partial^2}{\partial x^2}\right]\int_0^\infty dx\, e^{\frac{-\alpha x^2}{2}} \sin kx\right\}$$

$$= \frac{a\alpha\Omega}{(2\pi)^3} e^{\frac{-\alpha k^2}{2}} - \frac{2a^2\Omega(2\pi)^{1/2}}{\alpha k^2}\left[\frac{\partial}{\partial k} - \frac{1}{k}\right]\left[1 + \frac{1}{\alpha}\frac{\partial^2}{\partial k^2}\right]\left\{e^{\frac{-\alpha k^2}{2}}\int_0^{\sqrt{\alpha}k} dx\, e^{\frac{-x^2}{2}}\right\}$$

or

$$\alpha_{kk} = \Omega e^{\frac{-\alpha k^2}{2}}\left\{\langle \vec{k}|\vec{k}\rangle - \frac{\alpha a_0}{(2\pi)^3} + \frac{2a^2}{(2\pi)^{3/2}}\left[\frac{\alpha k^2 - 1}{k}\int_0^{\sqrt{\alpha}k} dx\, e^{\frac{x^2}{2}} - \sqrt{\alpha}\, e^{\frac{\alpha k^2}{2}}\right]\right\}$$

With the substitution of $\alpha_{kk}$ for the momentum diagonal matrix elements of $\mathcal{A}_t$ and $\mathcal{A}_{ts}$ above, equations (7.6) and (7.7) are obtained directly.

# APPENDIX F

## COMBINATORIAL FACTORS

In this appendix we show how to locate the parts of the expanded determinants which enter into equations (8.2). This involves the explicit functional form of the integrand as well as the combinatorial factor associated with the number of ways of obtaining equivalent terms.

It will be convenient to introduce the following simple diagrammatic notation for the terms to be considered. $a_{st}$ , $s \neq t$ is represented by a straight line labelled s and t at the two ends. Repeated subscripts are attached at their common point. $a_{ss}$ is represented by a dashed loop attached to the point labelled s . In this notation the term proportional to $a^2$ in equation (D.10) is shown in Fig. F.1.a. Those proportional to $a^3$ in equations (D.10) and (D.12) are shown in Fig. F.2.a. Complete consideration of n=2 would have turned up the additional terms indicated by the diagrams in Figures F.1.b and F.2.b.

The equivalence between the determinant notation of Appendix D and the diagram notation above is shown explicitly for n=3 in figures F.3 to F.10. The determinant shown is the one resulting from the angular integration

$$\int_0^{\pi} d\theta \sin\theta \, e^{i\vec{k}\cdot\vec{r}_{e'}} A_3(3) a_{e3} \qquad \text{(F.1)}$$

The general structure of $\psi^*\psi$ as the ratio of determinants leads to the following conclusions. There are n! equivalent terms $\sim a^n$ and having all n scattering indices. This corresponds to the n! ways of permuting the n indices among the n vertices excluding the fixed end points, e and e' (see figures F.3.b and F.4.b). There are two classes of terms $\sim a^{n+1}$ having all n scattering indices. There are the terms identical to those above except for the addition of a dashed loop. As there are n vertices available for the loop, there are n(n!) such terms (see figures F.3.a and F.4.a). Finally there are the terms which consist of a line of n' vertices between e and e' with an attached loop containing (n-n') vertices aside from the one shared with the line. For each n' such that $1 \leq n' \leq n-1$, there are n'(n!) equivalent diagrams. This can be seen as n! was of arranging the vertices, given a specific shared vertex for the loop and line, and n' choices for the shared vertex (see figures F.5.b to F.10.b).

The diagrams of figures (F.3.b) and (F.4.b) represent equivalent integrals, as do those of (F.3.c) and (F.4.c), (F.5) to (F.8) and (F.9) and (F.10). With the

aid of these figures, and recalling the definitions of equation (5.11.a) we see that

$$\int d\vec{k}\; \psi_k^*(\vec{r}_e;\vec{r}_1,\vec{r}_2,\vec{r}_3)\, e^{-\frac{\alpha k^2}{2}}\, \psi_k(\vec{r}_{e'};\vec{r}_1,\vec{r}_2,\vec{r}_3) \tag{F.2}$$

contributes

$$-4\pi a^3\, 3!\int_0^\infty dk\, k\, e^{-\frac{\alpha k^2}{2}}\, \frac{\sin k(r_{e1}+r_{12}+r_{23}+r_{3e'})}{r_{e1}\, r_{12}\, r_{23}\, r_{3e'}} \tag{F.3}$$

to $A_3(\alpha;a^3)$ and

$$-4\pi a^4\, 3!\int_0^\infty dk\, k\, e^{-\frac{\alpha k^2}{2}}\Big[3k\,\frac{\cos k(r_{e1}+r_{12}+r_{23}+r_{3e'})}{r_{e1}\, r_{12}\, r_{23}\, r_{3e'}}$$

$$+2\,\frac{\sin k(r_{e1}+r_{12}+2r_{23}+r_{2e'})}{r_{e1}\, r_{12}\, r_{23}^2\, r_{2e'}}$$

$$+\frac{\sin k(r_{e1}+r_{12}+r_{23}+r_{31}+r_{1e'})}{r_{e1}\, r_{12}\, r_{23}\, r_{31}\, r_{1e'}}\Big] \tag{F.4}$$

to $A_3(\alpha;a^4)$

# APPENDIX G

## INTEGRALS - ALL INDICES DISTINCT; $n^{th}$ ORDER

This appendix contains the integrations necessary to go from equation (8.5) to (8.7) and (8.9). The presentation is based on the work done by Coopersmith in his study of the free energy.[1] There the essential calculation was

$$tr \int\cdots\int \prod_{j=1}^{N} d\vec{r}_j \, e^{-\beta H(n)} \sim \int d\vec{r}_e \int\cdots\int \prod_{j=1}^{N} d\vec{r}_j \langle \vec{r}_e | e^{-\beta H(n)} | \vec{r}_e \rangle$$

where the trace was evaluated in coordinate representation. In the course of that analysis it was necessary to utilize the Fourier Integral Theorem. In our notation this is equivalent to

$$\int d\vec{r}_e \int\cdots\int \prod_{j=1}^{N} d\vec{r}_j \langle \vec{r}_e | e^{-\beta H(n)} | \vec{r}_{e'} \rangle$$

$$= \frac{1}{(2\pi)^3} \int d\vec{r}_{e'} \int d\vec{k} \int d\vec{r}_e \int\cdots\int \prod_{j=1}^{N} d\vec{r}_j \langle \vec{r}_e | e^{-\beta H(n)} | \vec{r}_{e'} \rangle \langle \vec{r}_{e'} | \vec{k} \rangle \langle \vec{k} | \vec{r}_e \rangle$$

$$= \int d\vec{k} \left\{ \frac{1}{(2\pi)^3} \int\cdots\int \prod_{j=1}^{N} d\vec{r}_j \langle \vec{k} | e^{-\beta H(n)} | \vec{k} \rangle \right\}$$

The bracketed expression appears as the basic building block for our present work. Therefore, we are able to adapt his solucions provided we are careful to select it in a form in which the final step (i.e. $\int d\vec{k}$ ) has not been taken.

Let us proceed to evaluate the integral obtained from equations (8.5) and (8.6).

$$R_n \equiv \frac{(-\rho a)^n n!\, e^{\frac{i't k^2}{2}}}{2\pi^2 \Omega} \int\cdots\int \prod_{j=1}^{n} d\vec{r}_j\, d\vec{r}_e\, d\vec{r}_{e'}\, \frac{e^{-i\vec{k}\cdot(\vec{r}_e - r_{e'})}}{r_{e1} r_{12} \cdots r_{n-1,n} r_{ne'}} \int_0^\infty dk'\, k' e^{-\frac{i't k'^2}{2}} \sin k's$$

where $s \equiv (r_{e1} + r_{12} + \cdots r_{n-1,n} + r_{ne'})$

First we consider

$$\int_0^\infty dk\, k\, e^{-\frac{\alpha k^2}{2}} \sin ks = -\frac{\partial}{\partial s}\int_0^\infty dk\, e^{-\frac{\alpha k^2}{2}} \cos ks = \frac{(\pi)^{1/2} s}{2^{1/2}(i't)^{3/2}} e^{\frac{-s^2}{2i't}}$$

This gives

$$R_n = \frac{B_n}{(4\pi)^{n+1}\Omega} \int\cdots\int \prod_{j=1}^{n} d\vec{r}_j\, d\vec{r}_e\, d\vec{r}_{e'}\, \frac{e^{-i\vec{k}\cdot(\vec{r}_e - \vec{r}_{e'})}}{r_{e1} r_{12} \cdots r_{n-1,n} r_{ne'}}\, s\, e^{\frac{-s^2}{2i't}}$$

$$B_n \equiv 2(2\pi)^{-1/2}(i't)^{-3/2} e^{\frac{i't k^2}{2}} (-4\pi\rho a)^n n!$$

As there are n+1 relative coordinates and n+2 variables of integration we can transform to new variables and redefine s

$$s = \sum_{j=1}^{n+1} r_j$$

$$R_n = B_n k^{-(n+1)} \int_0^\infty \cdots \int \prod_{j=1}^{n+1} d\vec{r}_j\, s\, e^{\frac{-s^2}{2i't}} \sin k r_j$$

The method of solution is as follows: It is clear that the effect of the n+1 integration could be expressed equally well by using a linear differential operator $f_k^{n+1}$ such that

$$R_n = \beta_n f_k^{n+1} k \exp(-itk^2/2)$$

It is therefore sufficient to find the effect of performing this operation. An equivalent expression for $k \exp(-itk^2/2)$ was seen above to be

$$k e^{-\frac{itk^2}{2}} = \frac{2}{(2\pi)^{1/2}(it)^{3/2}} \int_0^\infty ds \; s \, e^{\frac{-s^2}{2it}} \sin ks$$

so that we can let $u = s - r_1$ and write

$$R_n = B_n k^{-1} \int_0^\infty dr_1 \int_0^\infty du \; s \, e^{\frac{-s^2}{2it}} \sin kr_1 \, f_k^n \sin ku$$

$$= B_n \lim_{K \to k} k^{-1} f_k^n \int_0^\infty dr_1 \int_0^\infty du \; s \, e^{\frac{-s^2}{2it}} \sin Kr_1 \sin ku$$

$$= B_n \lim_{K \to k} (2K)^{-1} f_k^n \int_0^\infty ds \int_0^s dr \; s \, e^{\frac{-s^2}{2it}} \left\{ \cos[ks - (k+K)r] - \cos[ks + (K-k)r] \right\}$$

$$= B_n \lim_{K \to k} K^{-1} f_k^n \int_0^\infty ds \; s \, e^{\frac{-s^2}{2it}} (k^2 + K^2)^{-1} (k \sin Ks - K \sin ks)$$

$$= B_n \frac{(2\pi)^{1/2}(it)^{3/2}}{2} \lim_{K \to k} f_k^n k \, e^{-\frac{itk^2}{2}} \left( \frac{1 - e^{-\frac{it}{2}(K^2 - k^2)}}{K^2 - k^2} \right)$$

$$= B_n \frac{(2\pi)^{1/2}(it)^{3/2}}{2} \lim_{K \to k} \int_0^{\sqrt{it}} d\lambda \, \frac{\partial}{\partial \lambda} f_k^n k \, e^{-\frac{itk^2}{2}} \left( \frac{1 - e^{-\frac{\lambda^2}{2}(K^2 - k^2)}}{K^2 - k^2} \right)$$

$$= B_n \frac{(2\pi)^{1/2}(it)^{3/2}}{2} \lim_{K \to k} \int_0^{\sqrt{it}} d\lambda \, f_k^n k \, e^{-\frac{k^2}{2}(it - \lambda^2)} \, e^{-\frac{K^2\lambda^2}{2}}$$

Contemplating the initial expression defining $f_4^n$ we note that

$$f_4^n \, k \, e^{-\frac{it k^2}{2}} \equiv P_n(k^2, it) \equiv \sum_{j=1}^{n} a_n \frac{(it)^{j-1}}{k^{n-j}}$$

Thus,

$$R_n = B_n \frac{(2\pi)^{1/2}(it)^{3/2}}{2} e^{-\frac{it k^2}{2}} \int_0^{\sqrt{it}} d\lambda \, \lambda \, P_n(k^2, it-\lambda^2)$$

However, we also note that

$$\int_0^{\sqrt{it}} d\lambda \, \lambda \, P_n(k^2, it-\lambda^2) \equiv Q_n(k^2, it)$$

where $Q_n$ is also a polynomial with n terms. But $Q_{n-1}$ must equal $P_n$; therefore $P_n$ can contain only one non-zero term and from explicit consideration of $P_2$ (not shown here; see reference (1)) we see that this is the highest power of (it), namely $a_n(it)^{n-1}$. This gives the recursion relation

$$a_n = \frac{a_{n-1}}{2(n-1)}$$

so that we have

$$R_n = B_n \frac{(2\pi)^{1/2}(it)^{3/2}}{2} \cdot \frac{(it)^n e^{-\frac{it k^2}{2}}}{2^n n!} = (-2\pi\rho\alpha it)^n$$

In a similar manner we now evaluate the integral arising from equations (8.5) and (8.8.a)

$$S_n \equiv \frac{2a(-\rho a)^n n\,n!}{(2\pi)^2\,\Omega}\, e^{\frac{i't k^2}{2}} \int\cdots\int \prod_{j=1}^{n} d\vec{r}_j\, d\vec{r}_e\, d\vec{r}_{e'}\, \frac{e^{-i\vec{k}\cdot(\vec{r}_e-\vec{r}_{e'})}}{r_{e1}\, r_{12}\cdots r_{n-1,n}\, r_{ne'}} \int_0^\infty dk'\, k'\, e^{-\frac{i't k'^2}{2}} \cos k's$$

$$\int_0^\infty dk\, k^2 e^{-\frac{i't k^2}{2}} \cos ks = -\frac{\partial^2}{\partial s^2} \frac{(2\pi)^{1/2}}{2(i't)^{3/2}} e^{\frac{-s^2}{2i't}} = \frac{(2\pi)^{1/2}}{2(i't)^{3/2}} \left(2i't\frac{\partial}{\partial i't} - 1\right) e^{\frac{-s^2}{2i't}}$$

$$S_n = \frac{C_n}{(4\pi)^{n+1}\Omega} \int\cdots\int \prod_{j=1}^{n} d\vec{r}_j\, d\vec{r}_e\, d\vec{r}_{e'}\, \frac{e^{-i\vec{k}\cdot(\vec{r}_e-\vec{r}_{e'})}}{r_{e1}\, r_{12}\cdots r_{n-1,n}\, r_{ne'}}\, e^{\frac{-s^2}{2i't}}$$

$$C_n \equiv 2\,(i't)^{-3/2}(2\pi)^{-1/2}\, a\, e^{\frac{i't k^2}{2}} (-4\pi\rho a)^n\, n\, n!\, \left(2i't\frac{\partial}{\partial i't} - 1\right)$$

$$S_n = C_n\, k^{-(n+1)} \int\cdots\int \prod_{j=1}^{n+1} d\vec{r}_j\, e^{\frac{-s^2}{2i't}} \sin k r_j$$

$$= C_n\, f_k^{n+1} \int_0^\infty ds\, e^{\frac{-s^2}{2i't}} \sin ks$$

$$= C_n\, (i't)^{1/2} f_k^{n+1}\, e^{\frac{-i't k^2}{2}} \int_0^{k\sqrt{i't}} dx\, e^{\frac{x^2}{2}}$$

$$= C_n\, (i't)^{1/2} \int_0^{\sqrt{i't}} d\lambda\, \frac{\partial}{\partial\lambda} f_k^{n+1}\, e^{\frac{-k^2 i't}{2}} \int_0^{k\lambda} dx\, e^{\frac{x^2}{2}}$$

$$= C_n\, (i't)^{1/2} \int_0^{\sqrt{i't}} d\lambda\, f_k^{n+1}\, k\, e^{-\frac{k^2}{2}(i't-\lambda^2)}$$

$$= C_n\, (i't)^{1/2} \int_0^{\sqrt{i't}} d\lambda\, \frac{(i't-\lambda^2)^n}{2^n\, n!}\, e^{-\frac{k^2}{2}(i't-\lambda^2)}$$

$$= \frac{4\alpha n(-2\pi\rho a)^n}{(2\pi)^{1/2}} e^{\frac{k^2 it}{2}} \frac{\partial}{\partial(it)} \int_0^{\sqrt{it}} d\lambda (it-\lambda^2)^n e^{\frac{k^2}{2}(\lambda - it)}$$

The remaining integral is the one arising from equations (8.5) and (8.8.b)

$$T_n \equiv \frac{2\alpha(-\rho a)^n n!}{(2\pi)^2 \Omega} e^{\frac{it k^2}{2}} \sum_{m=1}^{n-1} m \int\cdots\int \prod_{j=1}^{n} d\vec{r}_j \, d\vec{r}_e \, d\vec{r}_{e'}$$

$$\times \frac{e^{-i\vec{k}\cdot(\vec{r}_e - \vec{r}_{e'})}}{r_{e1} r_{12} \cdots r_{m-1,m} r_{me'} r_{m,m+1} \cdots r_{n-1,n} r_{nm}} \int_0^\infty dk \, k e^{\frac{-itk^2}{2}} \sin ks$$

where now $s$ is defined by

$$s = (r_{e1} + r_{12} + \cdots r_{m-1,m} + r_{me'} + r_{m,m+1} + \cdots r_{n-1,n} + r_{nm})$$

$$T_n = \alpha B_n [\Omega (4\pi)^{n+1}] \sum_{m=1}^{n-1} \frac{m}{(2\pi)^3} \int\cdots\int d\vec{k} \, d\vec{r}_{n+1,m} \prod_{j=1}^{n} d\vec{r}_j \, d\vec{r}_e \, d\vec{r}_{e'}$$

$$\times \frac{e^{-i\vec{k}\cdot\vec{r}_{n+1,m}} e^{-i\vec{k}\cdot(\vec{r}_e - \vec{r}_{e'})}}{r_{e1} r_{12} \cdots r_{m-1,m} r_{me'} r_{m,m+1} \cdots r_{n-1,n} r_{n,m+1}} s e^{\frac{-s^2}{2it}}$$

$$= D_n \int\cdots\int \prod_{j=1}^{n+2} d\vec{r}_j \frac{\prod_{j=1}^{m+1} \sin k r_j}{k^{m+1}} \frac{\prod_{j=1}^{n+2} \sin K r_j}{K^{n+m+1}} s e^{\frac{-s^2}{2it}}$$

$$D_n \equiv \frac{\alpha B_n}{(2\pi)^3} \sum_{m=1}^{n-1} m \int d\vec{K}$$

$$T_n = D_n f_k^m f_K^{n-m} \int_0^\infty dr_1 \int_0^\infty dr_2 \, s e^{\frac{-s^2}{2it}} \sin k r_1 \sin K r_2$$

$$= -D_n \frac{(it)^{3/2}(2\pi)^{1/2}}{2} f_k^m f_k^{n-m} \frac{K k}{k^2-K^2} e^{-\frac{it k^2}{2}} \left(1 - e^{\frac{it}{2}(k^2-K^2)}\right)$$

$$= -D_n \frac{(it)^{3/2}(2\pi)^{1/2}}{2} \int_0^{\sqrt{it}} d\lambda \frac{\partial}{\partial \lambda} f_k^{n-m} f_k^m \frac{K k}{k^2-K^2} e^{-\frac{it k^2}{2}} \left(1 - e^{\frac{\lambda^2}{2}(k^2-K^2)}\right)$$

$$= -D_n \frac{(it)^{3/2}(2\pi)^{1/2}}{2} \int_0^{\sqrt{it}} d\lambda \, f_k^m f_k^{n-m} \, \lambda K k \, e^{\frac{-K^2\lambda^2}{2}} e^{-\frac{k^2}{2}(it-\lambda^2)}$$

$$= -D_n \frac{(it)^{3/2}(2\pi)^{1/2}}{2} \int_0^{\sqrt{it}} d\lambda \frac{\lambda^{2m-1}(it-\lambda^2)^{n-m-1}}{2^{n-2}(m-1)!(n-m-2)!} e^{\frac{-K^2\lambda^2}{2}} e^{-\frac{k^2}{2}(it-\lambda^2)}$$

$$= \frac{4a}{(2\pi)^3} \int_0^{\sqrt{it}} d\lambda \, e^{\frac{k^2\lambda^2}{2}} \sum_{m=1}^{n-1} \frac{n!(-2\pi\rho a)^m \lambda^{2m-1}(it-\lambda^2)^{n-m-1}}{(m-1)!\,(n-m-2)!} \int d\vec{k} \, e^{-\frac{K^2\lambda^2}{2}}$$

$$= \frac{-2a(-2\pi\rho a)^n n}{(2\pi)^{1/2}} \int_0^{\sqrt{it}} d\lambda \left[(it)^{n-1} - (\lambda^2)^{n-1}\right] e^{\frac{k^2\lambda^2}{2}}$$

## APPENDIX H

## SINGLE REPEATED INDEX; $n > 2$

We show in this appendix that where there are $n$ scattering interactions and only $m=n-1$ different scattering centers the corresponding $\mathcal{A}$ is separable to order $a^n$.

Let us consider a set $\{m\}$ of $m$ different indices divided into three subsets $\{m_1\}$, $\{m_2\}$ and $\{m_3\}$ such that $\{m_1\}$ and $\{m_3\}$ have one index in common. Thus $\{m_1\}$ contains the indices $1,2\ldots\nu\ldots m_1$; $m_2$ contains $m_1+1$, $m_1+2$, .... $m_1+m_2$; $m_3$ contains $m_1+m_2+1$, $m_1+m_2+2\ldots m,\nu$. This particular choice is convenient but not necessary for the results to be obtained. Specifically, we have to consider that part of $I$ which has all $n$ interactions represented and is proportional to $a^n$. $I$ is defined as

$$I \equiv \sum_{\nu} (P_{hh} \Omega^{m})^{-1} \int \cdots \int \prod_{j=1}^{m} d\vec{r}_j \langle \vec{h} | e^{-it\left(\frac{p^2}{2} + \sum_{\{m_1\}} V_j\right)} \left[ 1, e^{-\beta\left(\frac{p^2}{2} + \sum_{\{m_3\}} V_j\right)} \right] e^{it\left(\frac{p^2}{2} + \sum_{\{m_3\}} V_j\right)} | \vec{h} \rangle$$

$$\equiv \Sigma_{\nu} I_{\nu}$$

$I_{\nu}$ is represented diagramatically in figure H.1.a. The topographical factor associated with how many ways we can

obtain this integral for a given m is

$$\Sigma_J \equiv (m_1-1)!\sum_{J=1}^{m_1} m_2!\,(m_3-1)!\sum_{J=m_1,m_2+1}^{m_1+m_2+m_3}$$

$I_J$ can be rewritten as

$$I_J = \frac{1}{(2\pi)^3}\int\cdots\int\prod_{i=1}^{m+4} d\vec{r}_i \; e^{-i\vec{k}\cdot(\vec{r}_{m+1}-\vec{r}_{m+4})}$$

$$\times V(it,\{m_1\})_{m+1,m+2}(\vec{r}_{m+2}-\vec{r}_{m+3})\,V(\beta,\{m_2\})_{m+2,m+3}\,V(-it,\{m_3\})_{m+3,m+4}$$

where

$$V(\alpha,\{m\})_{n,n'} \equiv \langle \vec{r}_n | e^{-\alpha\left(\frac{p^2}{2}+\sum_{\{m\}} V_i\right)} | \vec{r}_{n'}\rangle$$

$$I_J = \frac{1}{(2\pi)^3}\int_{\vec{k}'\to\vec{k}}^{im} i\frac{\partial}{\partial k_i'}\int\cdots\int\prod_{i=1}^{m+4} d\vec{r}_i \; e^{-i\vec{k}\cdot(\vec{r}_{m+1}-\vec{r}_{m+2})} V(it,\{m_1\})_{m+1,m+2}$$

$$\times e^{-i\vec{k}'\cdot(\vec{r}_{m+2}-\vec{r}_{m+3})} V(\beta,\{m_2\})_{m+2,m+3}$$

$$\times e^{-i\vec{k}\cdot(\vec{r}_{m+3}-\vec{r}_{m+4})} V(-it,\{m_3\})_{m+3,m+4}$$

$$= \frac{1}{(2\pi)^6}\int_{\vec{k}'\to\vec{k}}^{im} i\frac{\partial}{\partial k_i'}\int\cdots\int\prod_{i=1}^{m+4} d\vec{r}_i\, d\vec{k}''\, d\vec{r}_{JJ'}\, e^{i\vec{k}''\cdot\vec{r}_{JJ'}}$$

$$\times e^{-i\vec{k}\cdot(\vec{r}_{m+1}-\vec{r}_{m+2})} V(it,\{m_1\})_{m+1,m+2}$$

$$\times e^{-i\vec{k}'\cdot(\vec{r}_{m+2}-\vec{r}_{m+3})} V(\beta,\{m_2\})_{m+2,m+3}$$

$$\times e^{-i\vec{k}\cdot(\vec{r}_{m+3}-\vec{r}_{m+4})} V(-it,\{m_3\})_{m+3,m+4}$$

where $\{m_3\}$ contains the indices $m_1+m_2+1$, $m_1+m_2+2, \ldots m, \nu$. In the last step we introduced a Fourier transform ("opened the ring") so that $I_\nu$ is now indicated diagrammatically in figure H.1.b. This figure also shows the transformation to relative coordinates which gives

$$I = \frac{\Omega}{\rho_{l'm'}(2\pi)^6} \delta_{\vec{A}'\to\vec{A}}\, i\frac{\partial}{\partial A_3'} \int d\vec{A}''\, I_{s_1}(\vec{A},\vec{A}'')\, I_{s_2}(\vec{A}',\vec{A}'')\, I_{s_3}(\vec{A},\vec{A}'')$$

$$I_{s_1}(\vec{A},\vec{A}'') \equiv \frac{(A_1-2)!}{\Omega^{s_1-1}} \sum_{j=1}^{s_1-1} \int\cdots\int \prod_{i=1}^{s_1} d\vec{r}_i\; e^{-i\vec{A}\cdot\sum_{i=1}^{j}\vec{r}_i - i(\vec{A}-\vec{A}'')\cdot\sum_{i=j+1}^{s_1}\vec{r}_i} V(it,\{s_1-1\})_{s_1}$$

$$I_{s_2}(\vec{A}',\vec{A}'') \equiv \frac{(s_2-1)!}{\Omega^{s_2-1}} \int\cdots\int \prod_{i=1}^{s_2} d\vec{r}_i\; e^{-i(\vec{A}'-\vec{A}'')\cdot\sum_{i=1}^{s_2}\vec{r}_i} V(\beta,\{s_2-1\})_{s_2}$$

$$I_{s_3}(\vec{A},\vec{A}'') \equiv \frac{(s_3-2)!}{\Omega^{s_3-1}} \sum_{j'=1}^{s_3-1} \int\cdots\int \prod_{i=1}^{s_3} d\vec{r}_i\; e^{-i(\vec{A}-\vec{A}'')\cdot\sum_{i=1}^{j'}\vec{r}_i - i\vec{A}\cdot\sum_{i=j'+1}^{s_3}\vec{r}_i} V(-it,\{s_3-1\})_{s_3}$$

The coordinate matrix elements are given by equation (7.6) which is this notation is $V(it,\{n\})_{e,e'}$, so that

$$I_{s_2} = \frac{(-1)^{s_2} a^{s_2-1}(4\pi)^{s_2}(s_2-1)!}{\Omega^{s_2-1}(2\pi)^{3/2}\beta^{3/2}(K')^{s_2}} \int_0^\infty\cdots\int \prod_{i=1}^{s_2} d\vec{r}_i\; \sin K' r_i \left(\sum_{i=1}^{s_2} r_i\right) e^{-\frac{\left(\sum_{i=1}^{s_2} r_i\right)^2}{2\beta}}$$

where $\vec{K}' = \vec{A}' - \vec{A}''$

This multiple integral is evaluated in Appendix G (as part of the evaluation of $R_n$) with the result

$$I_{s_2} = -4\pi\,(-2\pi a\beta/\Omega)^{s_2-1}\, e^{-\frac{\beta K'^2}{2}}$$

Similarly

$$I_{s_1} = \sum_{\nu=1}^{s_1-1} \frac{(s_1-2)!(-4\pi)^{s_1} a^{s_1-1}}{\Omega^{s_1-1}(2\pi)^{3/2}(it)^{3/2} k^{\nu} K^{s_1-\nu}} \int_0^{\infty}\cdots\int \prod_{j=1}^{s_1} dr_j \prod_{j=1}^{\nu} \sin k r_j \prod_{j=\nu+1}^{s_1} \sin K r_j \left(\sum_{j=1}^{s_1} r_j\right) e^{\frac{-\left(\sum_{j=1}^{s_1} r_j\right)^2}{2it}}$$

$$= \sum_{\nu=1}^{s_1-1} \frac{(s_1-2)!(-2\pi a)^{s_1-1} 4\pi}{\Omega^{s_1-1}} \int_0^{\sqrt{it}} d\lambda \, \frac{\lambda^{2\nu-1}(it-\lambda^2)^{s_1-\nu-1}}{(\nu-1)!(s_1-\nu-1)!} e^{-\frac{1}{2}k^2(it-\lambda^2)} e^{-\frac{K^2\lambda^2}{2}}$$

$$= \frac{-4\pi(s_1-2)!(-2\pi a)^{s_1-1}}{\Omega^{s_1-1}} \int_0^{\sqrt{it}} d\lambda \, e^{-\frac{k^2}{2}(it-\lambda^2)} e^{-\frac{K^2\lambda^2}{2}} \frac{\lambda}{s_1} \lim_{\lambda_1\to\lambda} \frac{\partial^2}{\partial(\lambda_1^2)^2} \sum_{\nu=2}^{s_1} \frac{s_1!(\lambda_1^2)^{\nu}(it-\lambda^2)^{s_1-\nu}}{(s_1-\nu)!\,\nu!}$$

$$= -4\pi(-2\pi a/\Omega)^{s_1-1} \int_0^{\sqrt{it}} d\lambda \, e^{-\frac{k^2}{2}(it-\lambda^2)} e^{-\frac{K^2\lambda^2}{2}} \lambda (it)^{s_1-2}$$

where $\vec{K} = (\vec{k}-\vec{k}'')$

The evaluation of $I_{s_3}$ is completely analogous to $I_{s_1}$ with $s_1$ replaced by $s_3$ and (it) replaced by (-it). When the above integrals are collected together we have

$$I = (-2\pi a\, it/\Omega)^{m_1-1} (-2\pi a\beta/\Omega)^{m_2} (-2\pi a\, it)^{m_3-1}$$

$$\times \frac{8a^2}{P_{44}(2\pi)^4} \lim_{\vec{k}'\to k} i\frac{\partial}{\partial k_3} \int d\vec{k}'' \left(\frac{1-e^{-\frac{it}{2}(K^2-k^2)}}{K^2-k^2}\right) e^{-\frac{\beta K'^2}{2}} \left(\frac{1-e^{-it(K^2-k^2)}}{K^2-k^2}\right)$$

Comparison of the coefficients on the upper line with equations (8.7) and (8.11) shows that the simply linked indices factorize and are therefore cumulantly separable. The lower line is the contribution from the

repeated index and the integral is the reclosing of the link at $\nu$.

## APPENDIX I

### SINGLE REPEATED SCATTERING INTERACTION $\sim \rho a^2$

In this appendix we look at that part of which is proportional to $a^2$ and contains the dual effect of $V_j$. This immediately restricts us to the product of functions of (it) and $\beta$, each proportional to one power of $a$.

For this appendix we define $A \equiv A(g_j(\alpha) g_j(\lambda))$

$$A \equiv (P_{kk'}\Omega)^{-1} \int d\vec{r}_j \langle \vec{k}' | e^{-it\left(\frac{p^2}{2}+V_j\right)} [\beta_j e^{-\beta\left(\frac{p^2}{2}+V_j\right)}] e^{\frac{it p^2}{2}} | \vec{k} \rangle \qquad (I.1)$$

$$= (P_{kk'}\Omega)^{-1} e^{\frac{it k^2}{2}} \int d\vec{r}_j \langle \vec{k}' | e^{-it\left(\frac{p^2}{2}+V_j\right)} e^{-\beta\left(\frac{p^2}{2}+V_j\right)} (-i) \int_0^\beta d\lambda\, e^{\lambda\left(\frac{p^2}{2}+V_j\right)} p_\beta e^{-\lambda\left(\frac{p^2}{2}+V_j\right)} | \vec{k} \rangle \qquad (I.2)$$

$$= -i (P_{kk'}\Omega)^{-1} e^{\frac{it k^2}{2}} \int d\vec{r}_j \int_0^\beta d\lambda \int d\vec{k}_1 \int d\vec{k}_2 \int d\vec{k}_3\, V(it)_{k k_1} V(\beta)_{k_1 k_2} V(-\lambda)_{k_2 k_3} k_{3_\beta} V(\lambda)_{k_3 k} \qquad (I.3)$$

$$V(\alpha)_{kk'} \equiv \langle \vec{k} | e^{-\alpha\left(\frac{p^2}{2}+V_j\right)} | \vec{k}' \rangle$$

$$= e^{-\frac{\alpha k'^2}{2}} \delta(\vec{k}-\vec{k}') - \frac{2\alpha}{(2\pi)^2} e^{-\frac{\alpha k'^2}{2}} \left( \frac{1 - e^{-\frac{\alpha}{2}(k'^2-k^2)}}{k'^2-k^2} \right) e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}_j}$$

$$A = \frac{-i\,4a^2}{P_{44}\,\Omega(2\pi)^4}\int d\vec{r}_j \int_0^{\beta} d\lambda \int\cdots\int d\vec{k}_1\, d\vec{k}_2\, d\vec{k}_3 \left(\frac{1-e^{-\frac{i\lambda t}{2}(k_1^2-k^2)}}{k_1^2-k^2}\right)$$

$$\times\Big[e^{-\frac{\beta k_2^2}{2}}\left(\frac{1-e^{-\frac{\beta}{2}(k_2^2-k_1^2)}}{k_2^2-k_1^2}\right)e^{-i(\vec{k}-\vec{k}_2)\cdot\vec{r}_j}e^{\frac{\lambda}{2}(k_3^2-k^2)}\delta(\vec{k}_1-\vec{k}_3)\,k_{3_y}\,\delta(\vec{k}_2-\vec{k})$$

$$+e^{-\frac{\beta k_2^2}{2}}\delta(\vec{k}_1-\vec{k}_2)\,e^{\frac{\lambda k_2^2}{2}}\left(\frac{1-e^{\frac{\lambda}{2}(k_3^2-k_1^2)}}{k_1^2-k_2^2}\right)e^{-i(\vec{k}_0-\vec{k}_1+\vec{k}_2-\vec{k}_3)\cdot\vec{r}_j}k_{3_y}\,e^{-\frac{\lambda k_3^2}{2}}\delta(\vec{k}_3-\vec{k})$$

$$+e^{-\frac{\beta k_2^2}{2}}\delta(\vec{k}_1-\vec{k}_2)\,e^{\frac{\lambda k_3^2}{2}}\delta(\vec{k}_2-\vec{k}_3)\,k_{3_y}\,e^{-\frac{\lambda k_3^2}{2}}\left(\frac{1-e^{-\frac{\lambda}{2}(k_2^2-k_3^2)}}{k_2^2-k_3^2}\right)e^{-i(\vec{k}_3-\vec{k}_1)\cdot\vec{r}_j}\Big] \qquad (I.4)$$

$$=\frac{-4ia^2}{(2\pi)^4 P_{44}}\int_0^{\beta}d\lambda\int d\vec{k}_1\left(\frac{1-e^{-\frac{it}{2}(k_1^2-k_0^2)}}{k_1^2-k^2}\right)\Big[e^{-\frac{\beta k_1^2}{2}}\left(\frac{1-e^{-\frac{\beta}{2}(k^2-k_1^2)}}{k^2-k_1^2}\right)k_{2_y}$$

$$+e^{-\frac{\beta k_1^2}{2}}e^{\frac{\lambda}{2}(k_1^2-k^2)}\left(\frac{1-e^{\frac{\lambda}{2}(k^2-k_1^2)}}{k^2-k_1^2}\right)k_{2_y}$$

$$+e^{-\frac{\beta k_1^2}{2}}k_{1_y}\left(\frac{1-e^{-\frac{\lambda}{2}(k^2-k_1^2)}}{k^2-k_1^2}\right)\Big] \qquad (I.5)$$

$$=\frac{-4ia^2}{(2\pi)^4 P_{44}}\int_0^{\beta}d\lambda\int d\vec{k}_1\Big\{e^{-\frac{\beta k_1^2}{2}}\int_0^{it}dx\,e^{-(k_1^2-k^2)\frac{x}{2}}$$

$$\times\Big[\int_0^{\alpha}dy\,e^{-(k^2-k_1^2)\frac{y}{2}}-\int_0^{\lambda}dy\,e^{-(k^2-k_1^2)\frac{y}{2}}\Big]\Big\} \qquad (I.6)$$

$$= \frac{-4ia^2k_2}{(2\pi)^4 P_{44}} \int_0^{it} dx \int_0^{\beta} dy\, e^{\frac{k^2}{2}(x-y)} \int d\vec{k}_1\, e^{-\frac{k_1^2}{2}(\beta-y+x)} \tag{I.7}$$

$$= \frac{-4ia^2k_2}{(2\pi)^{5/2} P_{44}} \int_0^{it} dx \int_0^{\beta} dy\, \frac{y\, e^{\frac{k^2}{2}(x-y)}}{(\beta-y+x)^{3/2}} \tag{I.8}$$

$$= \frac{-4ia^2k_2}{(2\pi)^{5/2} P_{44}} \int_0^{\beta} dq \int_{-q}^{it} dp\, \frac{q\, e^{\frac{k^2 p}{2}}}{(\beta+p)^{3/2}} \tag{I.9}$$

$$= \frac{-4ia^2k_2}{(2\pi)^{5/2} P_{44}} \left[ \int_0^{\beta} dp \int_p^{\beta} dq\, \frac{q\, e^{-\frac{k^2 p}{2}}}{(\beta-p)^{3/2}} + \int_0^{it} dp \int_0^{\beta} dq\, \frac{q\, e^{\frac{k^2 p}{2}}}{(\beta+p)^{3/2}} \right] \tag{I.10}$$

$$= \frac{-2ia^2k_2}{(2\pi)^{5/2} P_{44}} \left[ \int_0^{\beta} dp\, \frac{(\beta^2-p^2)\, e^{-\frac{k^2 p}{2}}}{(\beta-p)^{3/2}} + \beta^2 \int_0^{it} dp\, \frac{e^{\frac{k^2 p}{2}}}{(\beta+p)^{3/2}} \right] \tag{I.11}$$

In equation (I.2) we have introduced an identity for the commutator.[1] Equation (I.4) is obtained by taking one power of $a$ from $V(it)_{kk_1}$ and one power of $a$ from the product $V(\beta)_{k_1k_2} V(-\lambda)_{k_2k_3} V(\lambda)_{k_3k_1}$. The last term in (I.5) vanishes because of $k_{1z}$ which makes the integrand an odd function over the symmetric region of integration. The order of integration is changed in going from (I.6) to (I.7). (I.9) follows from (I.8) with the change of variables $x-y=p$, $y=q$. The complex integration in (I.9) is taken along the real axis from $(-q)$ to zero and along the imaginary axis from zero to $(it)$. A further interchange of the order of integrations gives (I.11).

# APPENDIX J

## SINGLE REPEATED SCATTERING INTERACTION; NON-CONTRIBUTING

We use the same technique as in Appendix I and select the term proportional to $a^2$ which contains both the (it) and (-it) aspects of the interaction.

$$\mathcal{A}(g_j(it)g_j(-it))$$

$$= (P_{kk}\Omega)^{-1}\int d\vec{r}_j \langle\vec{k}| e^{-it(\frac{p^2}{2}+V_j)}\left[\lambda, e^{-\frac{\beta p^2}{2}}\right] e^{it(\frac{p^2}{2}+V_j)}|\vec{k}\rangle$$

$$= i(P_{kk}\Omega)^{-1}\int d\vec{r}_j \int d\vec{k}'\, V(it)_{kk'}\left(\frac{\partial}{\partial k_j} e^{-\frac{\beta k'^2}{2}}\right) V(-it)_{k'k}$$

The above is clearly seen to vanish as soon as we recall (see Appendix I) that, in order a, $V(\alpha)_{kk'}$, is an even function of k and k' . This makes the integral over $d\vec{K}'$ vanish as a result of the oddness of its integrand.

# APPENDIX K

## STIRLING NUMBER[1] OF THE SECOND KIND

The multinomial coefficient $M_q$ is the number of ways of partitioning $q$ different objects into $m_k$ subsets each containing $k$ objects

$$M_q = \frac{q!}{\pi (k!)^{m_k} m_k!} \quad ; \sum_{k=1}^{q} k m_k = q$$

The Stirling number of the Second Kind $S_q^{(j)}$ is defined as

$$S_q^{(j)} \equiv \sum_{\substack{\Sigma k m_k = q \\ \Sigma m_k = j}} M_q$$

It satisfies the summation relation

$$\sum_{j=0}^{q} (-1)^{q-j} j!\, S_q^{(j)} = 1$$

Thus from equation (8.21) we have

$$\frac{n!}{(n-q)!} \sum_{j=0}^{q} (-1)^j j! \sum_{\substack{\Sigma k m_k = q \\ \Sigma m_k = j}} \frac{1}{\pi (k!)^{m_k} m_k!} = (-1)^q \frac{n!}{(n-q)!\, q!}$$

# APPENDIX L

## CUMULANT SUMMATION

Equation (8.23) is obtained from (8.22) as follows:

$$\mathcal{A}_n^c(\alpha;\alpha^{n+1}) = \sum_{k=1}^{\infty}\sum_{q=0}^{n} \mathcal{A}_{n-q}(\alpha;\alpha^{n-q+1})\left[\mathcal{A}_1(\alpha;\alpha)\right]^q \frac{(-1)^q}{(n-q)!\,q!}$$

$$= \frac{2a}{(2\pi)^{1/2}} \sum_{n=1}^{\infty}\sum_{q=0}^{n} (-R)^{n-q}(n-q)$$

$$\times \left\{ 2\frac{\partial}{\partial\alpha}\int_0^{\sqrt{\alpha}} d\lambda\,(it-\lambda^2)^{n-q} e^{-\frac{k^2}{2}(it-\lambda^2)} \right.$$

$$\left. + \int_0^{\sqrt{\alpha}} d\lambda \left[(it)^{n-q-1} - (\lambda^2)^{n-q-1}\right] e^{-\frac{k^2}{2}(it-\lambda^2)} \right\} \frac{R^q\, e^{\frac{it\,k^2}{2}}}{(n-q)!\,q!}$$

$$= \frac{2a}{(2\pi)^{1/2}} \sum_{n=1}^{\infty} \frac{R^n}{n!} \int_0^{\sqrt{\alpha}} d\lambda\, e^{\frac{k^2\lambda^2}{2}} \left[\Sigma_1 + \Sigma_2 + \Sigma_3 + \Sigma_4\right]$$

$$\Sigma_1 \equiv \sum_{q=0}^{n} \frac{2(n-q)^2\, n!}{(n-q)!\,q!} (-\alpha)^q (\alpha-\lambda^2)^{n-q-1}$$

$$= 2\frac{\partial}{\partial(-\lambda^2)} \sum_{q=0}^{n} \frac{(n-q)\,n!}{(n-q)!\,q!} (-\alpha)^q (\alpha-\lambda^2)^{n-q}$$

$$= 2\frac{\partial}{\partial(-\lambda^2)} \left[(\alpha-\lambda^2)\frac{\partial}{\partial(-\lambda^2)}(-\lambda^2)^n\right]$$

$$\Sigma_2 \equiv -k^2 \sum_{q=0}^{n} \frac{(n-q)\,n!}{(n-q)!\,q!} (-\alpha)^q (\alpha-\lambda^2)^{n-q}$$

$$= -k^2 (it - \lambda^2) \frac{\partial}{\partial(-\lambda^2)} (-\lambda^2)^n$$

$$\Sigma_3 \equiv - \sum_{\beta=0}^{n} \frac{(n-\beta)\, n!}{(n-\beta)!\, \beta!} (-1)^\beta \alpha^{n-1}$$

$$= - \lim_{\alpha' \to \alpha} \frac{\partial}{\partial \alpha'} \sum_{\beta=0}^{n} \frac{n!}{(n-\beta)!\, \beta!} (-\alpha)^\beta (\alpha')^{n-\beta}$$

$$= \begin{cases} 0 , & n > 1 \\ -1 , & n = 1 \end{cases}$$

$$\Sigma_4 \equiv \sum_{\beta=0}^{n} \frac{(n-\beta)\, n!}{(n-\beta)!\, \beta!} (-\alpha)^\beta (\lambda^2)^{n-\beta-1}$$

$$= \frac{\partial}{\partial(\lambda^2)} (\lambda^2 - \alpha)^n$$

$$A_n^c(\alpha; \alpha^{n+1}) = \frac{2a}{(2\pi)^{1/2}} \sum_{n=1}^{\infty} \left\{ \frac{(-R)^n}{n!} \int_0^{\sqrt{\alpha}} d\lambda\, e^{\frac{k^2\lambda^2}{2}} \left\{ \left(2\frac{\partial}{\partial(-\lambda^2)} - k^2\right) \left[ (\alpha - \lambda^2) \frac{\partial}{\partial(-\lambda^2)} (-\lambda^2)^n \right] \right.\right.$$
$$\left.\left. + \frac{\partial}{\partial(\lambda^2)} (\lambda^2 - \alpha)^n \right\}\right\} + \frac{2aR}{(2\pi)^{1/2}} \int_0^{\sqrt{\alpha}} d\lambda\, e^{\frac{\lambda^2 k^2}{2}}$$

$$= \frac{2a}{(2\pi)^{1/2}} \int_0^{\sqrt{\alpha}} d\lambda\, e^{\frac{k^2\lambda^2}{2}} \left\{ R + \left(2\frac{\partial}{\partial(-\lambda^2)} - k^2\right) \left[ (\alpha - \lambda^2) \frac{\partial}{\partial(-\lambda^2)} \sum_{n=1}^{\infty} \frac{(R\lambda^2)^n}{n!} \right] \right.$$
$$\left. + \frac{\partial}{\partial(\lambda^2)} \sum_{n=1}^{\infty} \frac{[R(\alpha - \lambda^2)]^n}{n!} \right\}$$

$$= \frac{2aR}{(2\pi)^{1/2}} \int_0^{\sqrt{\alpha}} d\lambda\, e^{\frac{k^2\lambda^2}{2}} \left[ 1 + (2R + k^2)(\alpha - \lambda^2) e^{R\lambda^2} - e^{R(\alpha - \lambda^2)} - 2 e^{R\lambda^2} \right]$$

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Appendix A

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Appendix G

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Appendix I

1. See reference (7), Section I

Appendix K

1. See reference (1), Section VI, Chap. 24

| Argument of $\mathscr{A}$ | N, $\Omega$, $\rho$ dependence | Contribution of $\mathscr{A}^c$ to $\mu$ | Location of discussion and calculation |
|---|---|---|---|
| $g_j(it)g_k(it)g_l(it)$<br>$g_j(\beta)g_k(\beta)g_l(\beta)$<br>$g_j(-it)g_k(-it)g_l(-it)$ | $\rho^3$ | $\sim\rho^3 a^4$ | Section VI, VII, VIII<br>Appendices E and F |
| $g_j^3(it)$ | $N/\Omega^3$ | None (levelled) | Section VI |
| $g_j^2(it)g_j(\beta)$ | | | |
| $g_j^2(it)g_j(-it)$ | | | |
| $g_j^3(\beta)$ | | | |
| $g_j(it)g_j^2(\beta)$ | | | |
| $g_j^2(\beta)g_j(-it)$ | | | |
| $g_j^3(-it)$ | | | |
| $g_j(it)g_j^2(-it)$ | | | |
| $g_j(\beta)g_j^2(-it)$ | | | |
| $g_j^2(it)g_k(it)$ | $N^2/\Omega^3$ | None (levelled) | Section VI |
| $g_j^2(it)g_k(\beta)$ | | | |
| $g_j^2(it)g_k(-it)$ | | | |
| $g_j(it)g_k^2(\beta)$ | | | |
| $g_j^2(\beta)g_k(\beta)$ | | | |
| $g_j^2(\beta)g_k(-it)$ | | | |
| $g_j(it)g_k^2(-it)$ | | | |
| $g_j(\beta)g_k^2(-it)$ | | | |
| $g_j(-it)g_k^2(-it)$ | | | |
| $g_j(it)g_k(\beta)g_l(-it)$ | $\rho^3$ | None (separable) | Section VI<br>Appendix I |
| $g_j(it)g_j(\beta)g_k(-it)$ | $\rho^2$ | None ( separable) | Section VI<br>Appendix I |
| $g_j(it)g_k(\beta)g_j(-it)$ | | | |
| $g_j(it)g_k(\beta)g_k(-it)$ | | | |
| $g_j(it)g_j(\beta)g_j(-it)$ | $\rho$ | None ($\sim\rho a^3$) | Section VI |

Figure 7.1 - A listing of all $n = 3$ terms arising from the expansion of $\mu$ by cumulants.

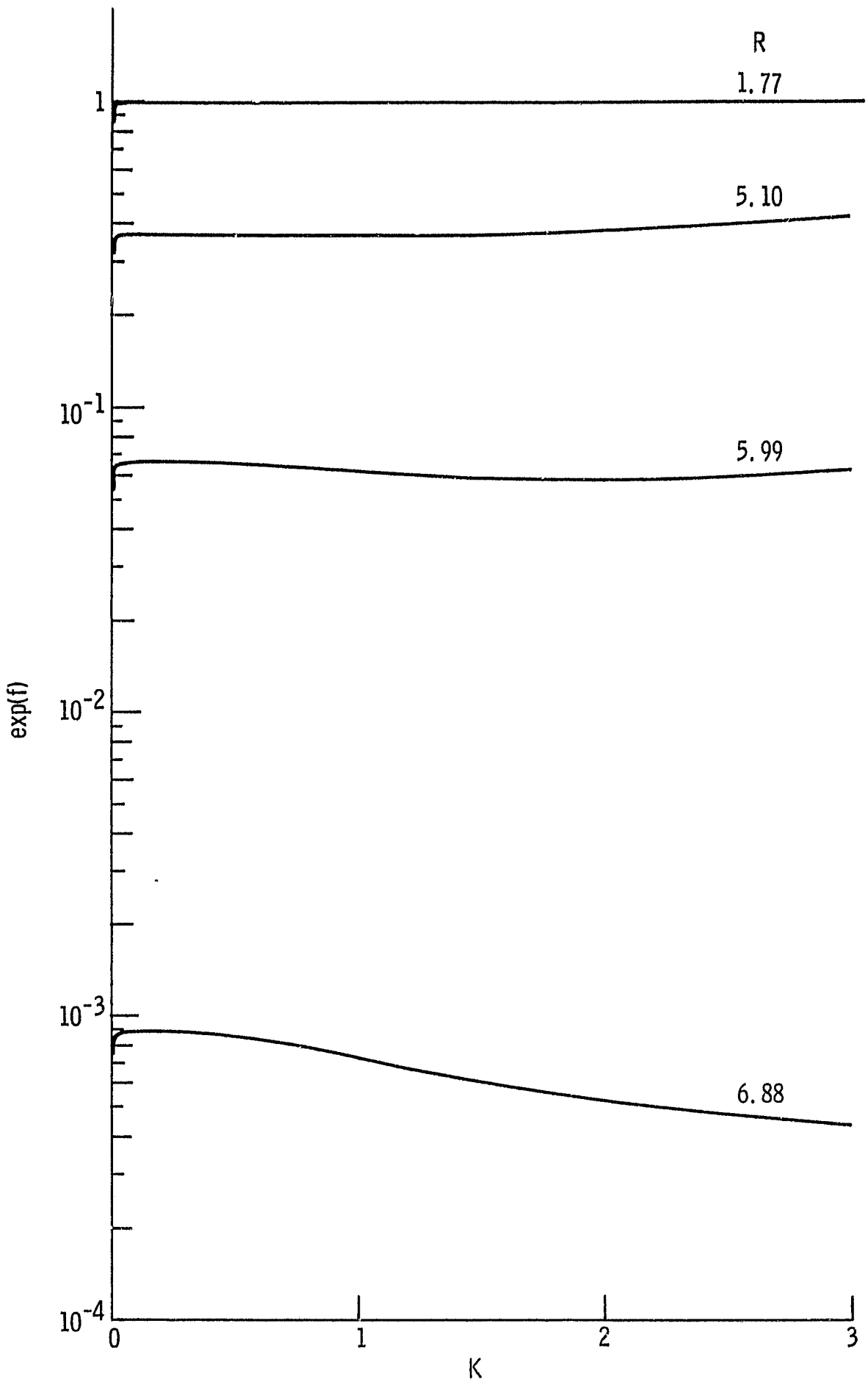



Figure 9.1 - exp(f) versus K for four values of R.

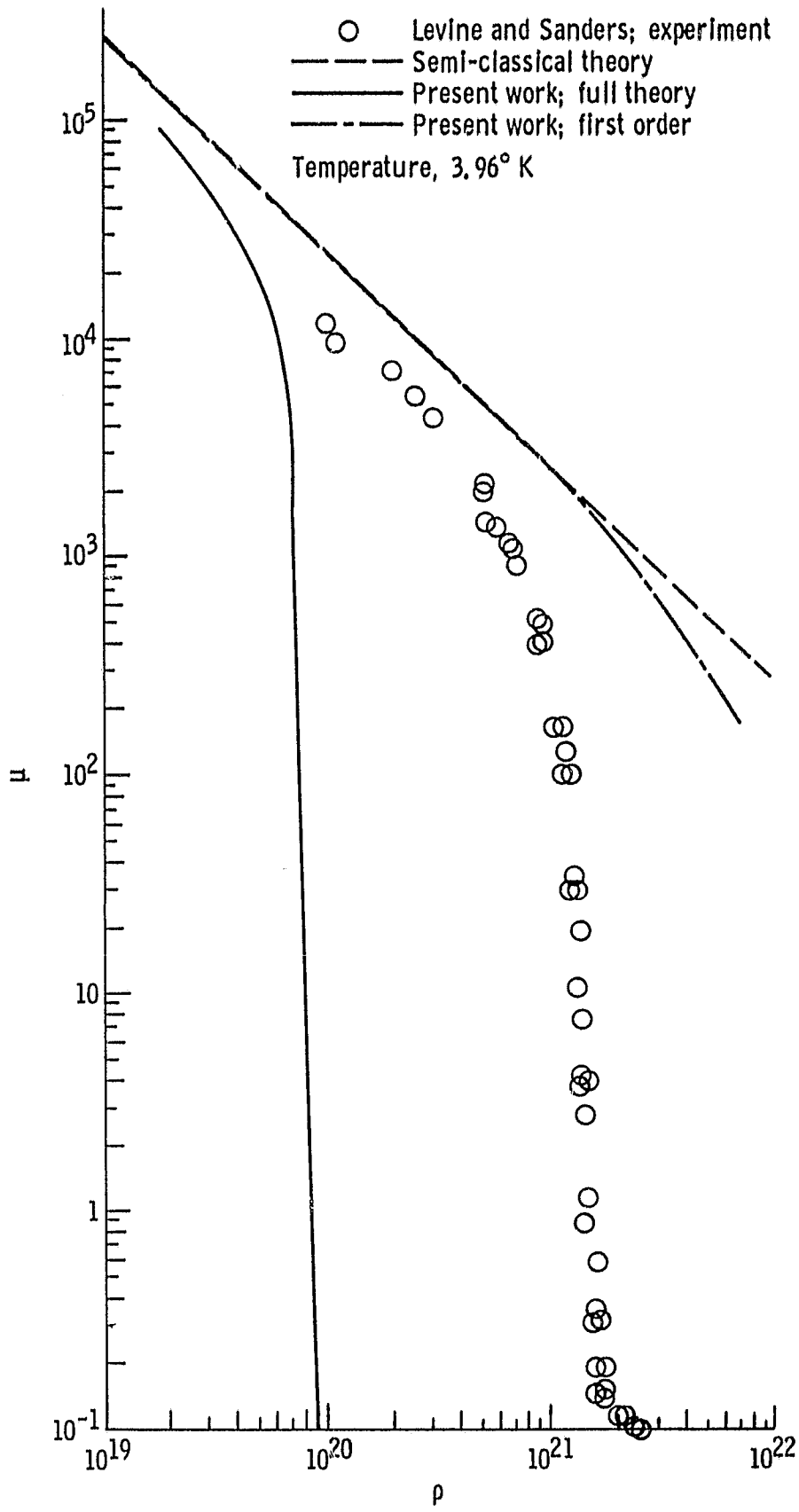



Figure 9.2 - Mobility μ ($cm^2$/Vsec) versus number density ρ ($atoms/cm^3$) at constant temperature for a = 0.62 Å.


Figure F.1 - (a) Diagram corresponding to equation (D 12). (b) Equivalent diagram for n = 2, not considered in Appendix D.

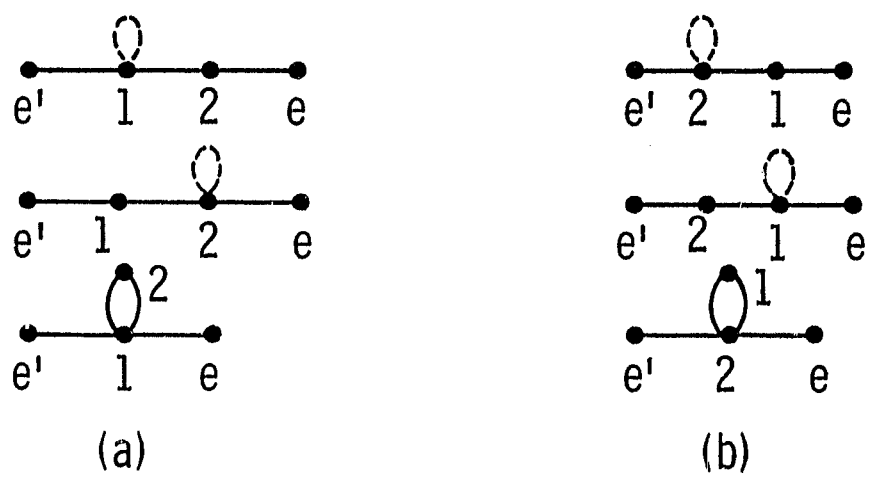
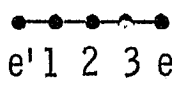



Figure F.2 - (a) Diagrams corresponding to equations (D.11) and (D.13). (b) Equivalent diagrams for n = 2, not considered in Appendix D.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} 1 + a_{11} & a_{12} & \boxed{a_{e'1}} - a^{*}_{e'1} \\ \boxed{a_{21}} & 1 + a_{22} & a_{e'2} - a^{*}_{e'2} \\ a_{31} & \boxed{a_{32}} & a_{e'3} - a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} \boxed{1 + a_{11}} & a_{12} & a_{13} \\ a_{21} & \boxed{1 + a_{22}} & a_{23} \\ a_{31} & a_{32} & \boxed{1 + a_{33}} \end{vmatrix}}$$

(a)



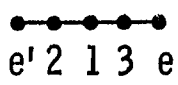

(b)


(a)

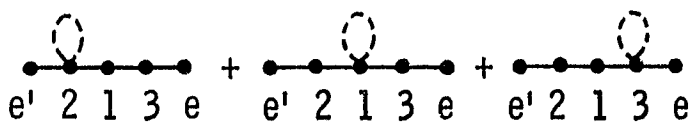
Figure F.3 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$. (c) Equivalent diagram notation for term $\sim a^4$.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} 1 + a_{11} & \boxed{a_{12}} & a_{e'1} - a^{*}_{e'1} \\ a_{21} & 1 + a_{22} & \boxed{a_{e'2}} - a^{*}_{e'2} \\ \boxed{a_{31}} & a_{32} & a_{e'3} - a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} \boxed{1 + a_{11}} & a_{12} & a_{13} \\ a_{21} & \boxed{1 + a_{22}} & a_{23} \\ a_{31} & a_{32} & \boxed{1 + a_{33}} \end{vmatrix}}$$

(a)




(b)

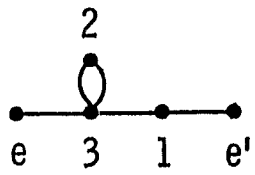



(c)

Figure F.4 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$. (c) Equivalent diagram notation for term $\sim a^4$.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} 1 + a_{11} & a_{12} & \boxed{a_{e'1}} - a^{*}_{e'1} \\ a_{21} & \boxed{1} + a_{22} & a_{e'2} - a^{*}_{e'2} \\ \boxed{a_{31}} & a_{32} & a_{e'3} - a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} \boxed{1} + a_{11} & a_{12} & a_{13} \\ a_{21} & 1 + a_{22} & \boxed{a_{23}} \\ a_{31} & \boxed{a_{32}} & 1 + a_{33} \end{vmatrix}}$$

(a)

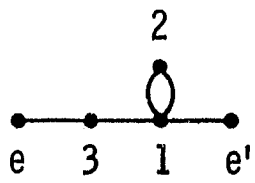



(b)

Figure F.5 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} 1 + a_{11} & a_{12} & \boxed{a_{e'1}} - a^{*}_{e'1} \\ a_{21} & \boxed{1} + a_{22} & a_{e'2} - a^{*}_{e'2} \\ \boxed{a_{31}} & a_{32} & a_{e'3} - a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} 1 + a_{11} & \boxed{a_{12}} & a_{13} \\ \boxed{a_{21}} & 1 + a_{22} & a_{23} \\ a_{31} & a_{32} & \boxed{1} + a_{33} \end{vmatrix}}$$

(a)

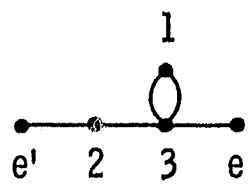



(b)

Figure F.6 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} \boxed{1}+a_{11} & a_{12} & a_{e'1}-a^{*}_{e'1} \\ a_{21} & 1+a_{22} & \boxed{a_{e'2}}-a^{*}_{e'2} \\ a_{31} & \boxed{a_{32}} & a_{e'3}-a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} 1+a_{11} & a_{12} & \boxed{a_{13}} \\ a_{21} & \boxed{1}+a_{22} & a_{23} \\ \boxed{a_{31}} & a_{32} & 1+a_{33} \end{vmatrix}}$$

(a)

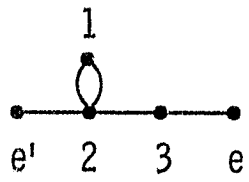



(b)

Figure F.7 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} \boxed{1} + a_{11} & a_{12} & a_{e'1} - a^{*}_{e'1} \\ a_{21} & 1 + a_{22} & \boxed{a_{e'2}} - a^{*}_{e'2} \\ a_{31} & \boxed{a_{32}} & a_{e'3} - a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} 1 + a_{11} & \boxed{a_{12}} & a_{13} \\ \boxed{a_{21}} & 1 + a_{22} & a_{23} \\ a_{31} & a_{32} & \boxed{1} + a_{33} \end{vmatrix}}$$

(a)

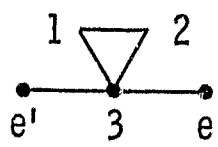



(b)

Figure F.8 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$.

$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} \boxed{1} + a_{11} & a_{12} & a_{e'1} - a^{*}_{e'1} \\ a_{21} & \boxed{1} + a_{22} & a_{e'2} - a^{*}_{e'2} \\ a_{31} & a_{32} & \boxed{a_{e'3}} - a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} 1 + a_{11} & \boxed{a_{12}} & a_{13} \\ a_{21} & 1 + a_{22} & \boxed{a_{23}} \\ \boxed{a_{31}} & a_{32} & 1 + a_{33} \end{vmatrix}}$$

(a)

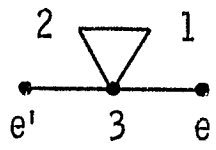



(b)

Figure F.9 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E.4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$.

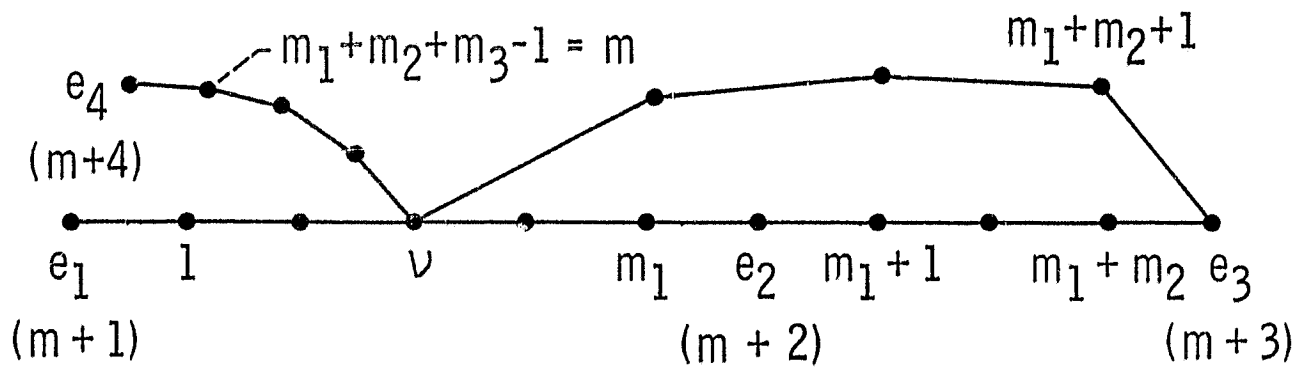
$$\frac{-a_{e3}}{ika} \times \frac{\begin{vmatrix} \boxed{1}+a_{11} & a_{12} & a_{e'1}-a^{*}_{e'1} \\ a_{21} & \boxed{1}+a_{22} & a_{e'2}-a^{*}_{e'2} \\ a_{31} & a_{32} & \boxed{a_{e'3}}-a^{*}_{e'3} \end{vmatrix}}{\begin{vmatrix} 1+a_{11} & a_{12} & \boxed{a_{13}} \\ \boxed{a_{21}} & 1+a_{22} & a_{23} \\ a_{31} & \boxed{a_{32}} & 1+a_{33} \end{vmatrix}}$$

(a)

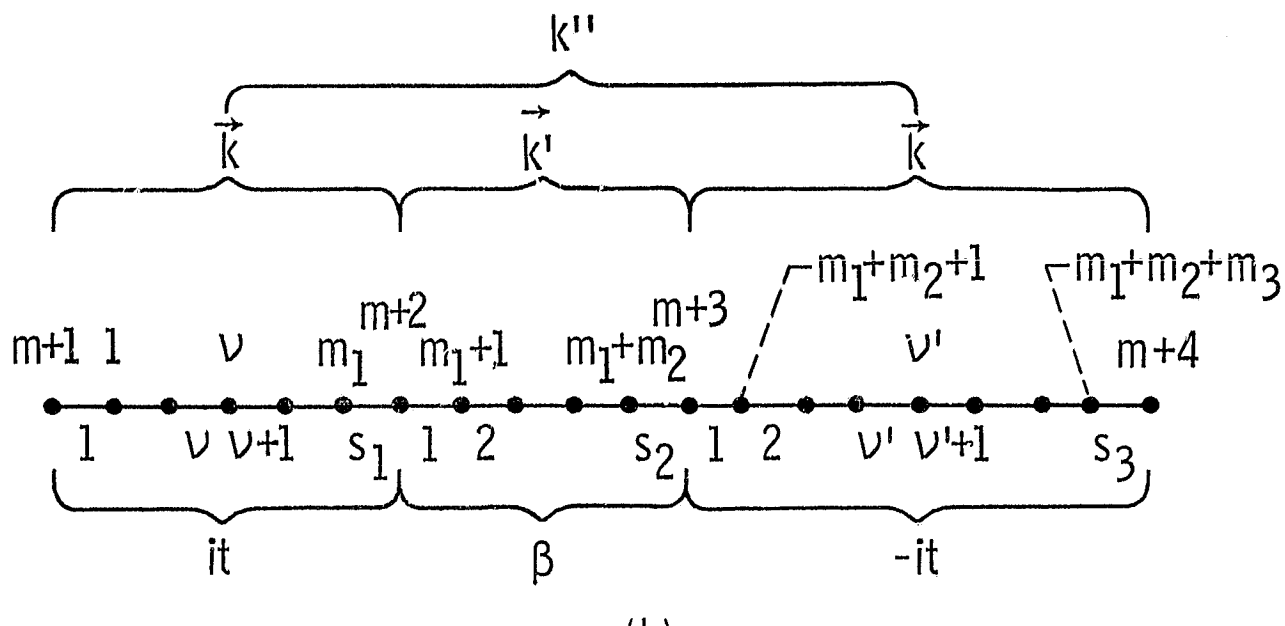



(b)

Figure F. 10 - (a) Schematic notation whereby the elements of the determinant which contibute to equation (E. 4) are indicated by encirclement. (b) Equivalent diagram notation for term $\sim a^3$.




(a)




(b)

Figure H. 1 - Diagram representation of $I_\nu$. (a) Initially. (b) After the Fourier transform.